



# Full wwPDB EM Validation Report ⓘ

Feb 20, 2023 – 03:35 pm GMT

PDB ID : 7PIW  
EMDB ID : EMD-13455  
Title : Stacked stretched Dunaliella PSII  
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.  
Deposited on : 2021-08-23  
Resolution : 4.00 Å (reported)  
Based on initial model : 6KAC

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

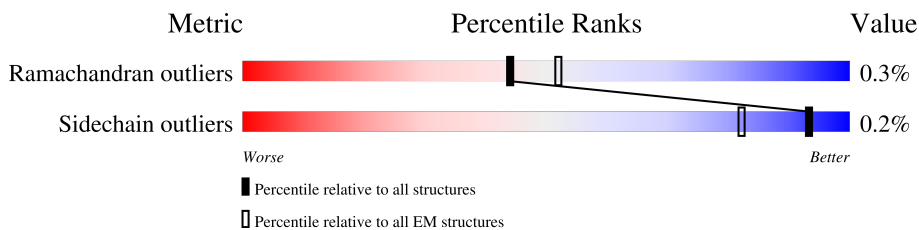
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	31% 99% .
1	A1	336	16% 100%
1	a	336	37% 99% .
1	a1	336	42% 99% .
2	B	484	53% 99% .
2	B1	484	16% 100%
2	b	484	56% 100%
2	b1	484	33% 100%
3	V	32	59% 100%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	V1	32	28% 100%
3	v	32	84% 100%
3	v1	32	66% 100%
4	C	449	28% 99%
4	C1	449	11% 100%
4	c	449	46% 99%
4	c1	449	36% 99%
5	D	348	41% 99%
5	D1	348	18% 100%
5	d	348	41% 99%
5	d1	348	43% 99%
6	E	76	58% 100%
6	E1	76	12% 100%
6	e	76	75% 100%
6	e1	76	45% 100%
7	F	31	45% 100%
7	F1	31	. 100%
7	f	31	65% 100%
7	f1	31	29% 100%
8	H	67	70% 97%
8	H1	67	34% 100%
8	h	67	78% 99%
8	h1	67	46% 99%
9	I	35	40% 100%
9	I1	35	20% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
9	i	35	37%	100%
9	i1	35	46%	100%
10	J	36	39%	100%
10	J1	36	36%	100%
10	j	36	72%	100%
10	j1	36	47%	100%
11	K	37	51%	97%
11	K1	37	19%	97%
11	k	37	57%	100%
11	k1	37	46%	100%
12	L	38	53%	97%
12	L1	38	39%	100%
12	l	38	50%	100%
13	M	32	62%	97%
13	m	32	84%	97%
14	O	238	79%	98%
14	O1	238	24%	98%
14	o	238	82%	98%
14	o1	238	33%	98%
15	P	187	100%	99%
15	P1	187	94%	99%
15	p	187	100%	100%
15	p1	187	93%	100%
16	T	30	53%	97%
16	T1	30	40%	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	t	30	53% 97%
16	t1	30	63% 100%
17	W	44	68% 98%
17	W1	44	14% 98%
17	w	44	59% 100%
17	w1	44	41% 100%
18	X	30	73% 100%
18	X1	30	20% 100%
18	x	30	73% 100%
18	x1	30	60% 100%
19	Z	61	75% 100%
19	Z1	61	15% 100%
19	z	61	92% 100%
19	z1	61	46% 100%
20	N	222	65% 99%
20	N1	222	9% 100%
20	n	222	88% 98%
20	n1	222	26% 100%
21	G	221	83% 99%
21	G1	221	10% 100%
21	g	221	89% 99%
21	g1	221	23% 100%
22	R	202	97% 100%
22	r	202	94% 100%
23	S	243	77% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
23	S1	243	9% 98%
23	s	243	87% 99%
23	s1	243	44% 98%
24	Y	222	56% 98%
24	Y1	222	11% 100%
24	y	222	64% 99%
24	y1	222	27% 99%
25	U	27	89% 100%
25	U1	27	41% 100%
25	u	27	78% 100%
25	u1	27	52% 93% 7%
26	M1	31	65% 100%
26	m1	31	55% 100%
27	R1	202	39% 97%
27	r1	202	41% 96%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	A	405	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	A	407	X	-	-	-
31	CLA	A	410	X	-	-	-
31	CLA	A1	405	X	-	-	-
31	CLA	A1	406	X	-	-	-
31	CLA	A1	407	X	-	-	-
31	CLA	A1	410	X	-	-	-
31	CLA	B	602	X	-	-	-
31	CLA	B	603	X	-	-	-
31	CLA	B	604	X	-	-	-
31	CLA	B	605	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	609	X	-	-	-
31	CLA	B	610	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	B	617	X	-	-	-
31	CLA	B1	602	X	-	-	-
31	CLA	B1	603	X	-	-	-
31	CLA	B1	604	X	-	-	-
31	CLA	B1	605	X	-	-	-
31	CLA	B1	606	X	-	-	-
31	CLA	B1	607	X	-	-	-
31	CLA	B1	608	X	-	-	-
31	CLA	B1	609	X	-	-	-
31	CLA	B1	610	X	-	-	-
31	CLA	B1	611	X	-	-	-
31	CLA	B1	612	X	-	-	-
31	CLA	B1	613	X	-	-	-
31	CLA	B1	614	X	-	-	-
31	CLA	B1	615	X	-	-	-
31	CLA	B1	616	X	-	-	-
31	CLA	B1	617	X	-	-	-
31	CLA	C	501	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C1	501	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	C1	502	X	-	-	-
31	CLA	C1	503	X	-	-	-
31	CLA	C1	504	X	-	-	-
31	CLA	C1	505	X	-	-	-
31	CLA	C1	506	X	-	-	-
31	CLA	C1	507	X	-	-	-
31	CLA	C1	508	X	-	-	-
31	CLA	C1	509	X	-	-	-
31	CLA	C1	510	X	-	-	-
31	CLA	C1	511	X	-	-	-
31	CLA	C1	512	X	-	-	-
31	CLA	C1	513	X	-	-	-
31	CLA	D	402	X	-	-	-
31	CLA	D	403	X	-	-	-
31	CLA	D1	402	X	-	-	-
31	CLA	D1	403	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	G	614	X	-	-	-
31	CLA	G1	602	X	-	-	-
31	CLA	G1	603	X	-	-	-
31	CLA	G1	604	X	-	-	-
31	CLA	G1	610	X	-	-	-
31	CLA	G1	611	X	-	-	-
31	CLA	G1	612	X	-	-	-
31	CLA	G1	613	X	-	-	-
31	CLA	G1	614	X	-	-	-
31	CLA	N	602	X	-	-	-
31	CLA	N	603	X	-	-	-
31	CLA	N	604	X	-	-	-
31	CLA	N	610	X	-	-	-
31	CLA	N	611	X	-	-	-
31	CLA	N	612	X	-	-	-
31	CLA	N	613	X	-	-	-
31	CLA	N	614	X	-	-	-
31	CLA	N1	602	X	-	-	-
31	CLA	N1	603	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	N1	604	X	-	-	-
31	CLA	N1	610	X	-	-	-
31	CLA	N1	611	X	-	-	-
31	CLA	N1	612	X	-	-	-
31	CLA	N1	613	X	-	-	-
31	CLA	N1	614	X	-	-	-
31	CLA	R	602	X	-	-	-
31	CLA	R	603	X	-	-	-
31	CLA	R	604	X	-	-	-
31	CLA	R	608	X	-	-	-
31	CLA	R	609	X	-	-	-
31	CLA	R	610	X	-	-	-
31	CLA	R	611	X	-	-	-
31	CLA	R	612	X	-	-	-
31	CLA	R	613	X	-	-	-
31	CLA	R1	602	X	-	-	-
31	CLA	R1	603	X	-	-	-
31	CLA	R1	604	X	-	-	-
31	CLA	R1	608	X	-	-	-
31	CLA	R1	609	X	-	-	-
31	CLA	R1	610	X	-	-	-
31	CLA	R1	612	X	-	-	-
31	CLA	S	602	X	-	-	-
31	CLA	S	603	X	-	-	-
31	CLA	S	604	X	-	-	-
31	CLA	S	605	X	-	-	-
31	CLA	S	609	X	-	-	-
31	CLA	S	610	X	-	-	-
31	CLA	S	611	X	-	-	-
31	CLA	S	612	X	-	-	-
31	CLA	S	613	X	-	-	-
31	CLA	S	614	X	-	-	-
31	CLA	S	617	X	-	-	-
31	CLA	S1	602	X	-	-	-
31	CLA	S1	603	X	-	-	-
31	CLA	S1	604	X	-	-	-
31	CLA	S1	605	X	-	-	-
31	CLA	S1	609	X	-	-	-
31	CLA	S1	610	X	-	-	-
31	CLA	S1	611	X	-	-	-
31	CLA	S1	612	X	-	-	-
31	CLA	S1	613	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	S1	614	X	-	-	-
31	CLA	S1	617	X	-	-	-
31	CLA	Y	602	X	-	-	-
31	CLA	Y	603	X	-	-	-
31	CLA	Y	604	X	-	-	-
31	CLA	Y	608	X	-	-	-
31	CLA	Y	610	X	-	-	-
31	CLA	Y	611	X	-	-	-
31	CLA	Y	612	X	-	-	-
31	CLA	Y	613	X	-	-	-
31	CLA	Y	614	X	-	-	-
31	CLA	Y1	602	X	-	-	-
31	CLA	Y1	603	X	-	-	-
31	CLA	Y1	604	X	-	-	-
31	CLA	Y1	608	X	-	-	-
31	CLA	Y1	610	X	-	-	-
31	CLA	Y1	611	X	-	-	-
31	CLA	Y1	612	X	-	-	-
31	CLA	Y1	613	X	-	-	-
31	CLA	Y1	614	X	-	-	-
31	CLA	a	405	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	a	410	X	-	-	-
31	CLA	a1	405	X	-	-	-
31	CLA	a1	406	X	-	-	-
31	CLA	a1	407	X	-	-	-
31	CLA	a1	410	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	610	X	-	-	-
31	CLA	b	611	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	b	616	X	-	-	-
31	CLA	b	617	X	-	-	-
31	CLA	b1	602	X	-	-	-
31	CLA	b1	603	X	-	-	-
31	CLA	b1	604	X	-	-	-
31	CLA	b1	605	X	-	-	-
31	CLA	b1	606	X	-	-	-
31	CLA	b1	607	X	-	-	-
31	CLA	b1	608	X	-	-	-
31	CLA	b1	609	X	-	-	-
31	CLA	b1	610	X	-	-	-
31	CLA	b1	611	X	-	-	-
31	CLA	b1	612	X	-	-	-
31	CLA	b1	613	X	-	-	-
31	CLA	b1	614	X	-	-	-
31	CLA	b1	615	X	-	-	-
31	CLA	b1	616	X	-	-	-
31	CLA	b1	617	X	-	-	-
31	CLA	c	501	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-
31	CLA	c	513	X	-	-	-
31	CLA	c1	501	X	-	-	-
31	CLA	c1	502	X	-	-	-
31	CLA	c1	503	X	-	-	-
31	CLA	c1	504	X	-	-	-
31	CLA	c1	505	X	-	-	-
31	CLA	c1	506	X	-	-	-
31	CLA	c1	507	X	-	-	-
31	CLA	c1	508	X	-	-	-
31	CLA	c1	509	X	-	-	-
31	CLA	c1	510	X	-	-	-
31	CLA	c1	511	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c1	512	X	-	-	-
31	CLA	c1	513	X	-	-	-
31	CLA	d	402	X	-	-	-
31	CLA	d	403	X	-	-	-
31	CLA	d1	402	X	-	-	-
31	CLA	d1	403	X	-	-	-
31	CLA	g	602	X	-	-	-
31	CLA	g	603	X	-	-	-
31	CLA	g	604	X	-	-	-
31	CLA	g	610	X	-	-	-
31	CLA	g	611	X	-	-	-
31	CLA	g	612	X	-	-	-
31	CLA	g	613	X	-	-	-
31	CLA	g	614	X	-	-	-
31	CLA	g1	602	X	-	-	-
31	CLA	g1	603	X	-	-	-
31	CLA	g1	604	X	-	-	-
31	CLA	g1	610	X	-	-	-
31	CLA	g1	611	X	-	-	-
31	CLA	g1	612	X	-	-	-
31	CLA	g1	613	X	-	-	-
31	CLA	g1	614	X	-	-	-
31	CLA	n	602	X	-	-	-
31	CLA	n	603	X	-	-	-
31	CLA	n	604	X	-	-	-
31	CLA	n	610	X	-	-	-
31	CLA	n	611	X	-	-	-
31	CLA	n	612	X	-	-	-
31	CLA	n	613	X	-	-	-
31	CLA	n	614	X	-	-	-
31	CLA	n1	602	X	-	-	-
31	CLA	n1	603	X	-	-	-
31	CLA	n1	604	X	-	-	-
31	CLA	n1	610	X	-	-	-
31	CLA	n1	611	X	-	-	-
31	CLA	n1	612	X	-	-	-
31	CLA	n1	613	X	-	-	-
31	CLA	n1	614	X	-	-	-
31	CLA	r	602	X	-	-	-
31	CLA	r	603	X	-	-	-
31	CLA	r	604	X	-	-	-
31	CLA	r	608	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	r	609	X	-	-	-
31	CLA	r	610	X	-	-	-
31	CLA	r	611	X	-	-	-
31	CLA	r	612	X	-	-	-
31	CLA	r	613	X	-	-	-
31	CLA	r1	602	X	-	-	-
31	CLA	r1	603	X	-	-	-
31	CLA	r1	604	X	-	-	-
31	CLA	r1	608	X	-	-	-
31	CLA	r1	609	X	-	-	-
31	CLA	r1	610	X	-	-	-
31	CLA	r1	612	X	-	-	-
31	CLA	s	602	X	-	-	-
31	CLA	s	603	X	-	-	-
31	CLA	s	604	X	-	-	-
31	CLA	s	605	X	-	-	-
31	CLA	s	609	X	-	-	-
31	CLA	s	610	X	-	-	-
31	CLA	s	611	X	-	-	-
31	CLA	s	612	X	-	-	-
31	CLA	s	613	X	-	-	-
31	CLA	s	614	X	-	-	-
31	CLA	s	617	X	-	-	-
31	CLA	s1	602	X	-	-	-
31	CLA	s1	603	X	-	-	-
31	CLA	s1	604	X	-	-	-
31	CLA	s1	605	X	-	-	-
31	CLA	s1	609	X	-	-	-
31	CLA	s1	610	X	-	-	-
31	CLA	s1	611	X	-	-	-
31	CLA	s1	612	X	-	-	-
31	CLA	s1	613	X	-	-	-
31	CLA	s1	614	X	-	-	-
31	CLA	s1	617	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	608	X	-	-	-
31	CLA	y	610	X	-	-	-
31	CLA	y	611	X	-	-	-
31	CLA	y	612	X	-	-	-
31	CLA	y	613	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	y	614	X	-	-	-
31	CLA	y1	602	X	-	-	-
31	CLA	y1	603	X	-	-	-
31	CLA	y1	604	X	-	-	-
31	CLA	y1	608	X	-	-	-
31	CLA	y1	610	X	-	-	-
31	CLA	y1	611	X	-	-	-
31	CLA	y1	612	X	-	-	-
31	CLA	y1	613	X	-	-	-
31	CLA	y1	614	X	-	-	-
37	C7Z	B	620	X	-	-	-
37	C7Z	B1	620	X	-	-	-
37	C7Z	b	620	X	-	-	-
37	C7Z	b1	620	X	-	-	-
42	LMK	C	527	X	-	-	-
42	LMK	C1	527	X	-	-	-
42	LMK	c	627	X	-	-	-
42	LMK	c1	527	X	-	-	-
46	RRX	H	101	X	-	-	-
46	RRX	H1	101	X	-	-	-
46	RRX	h	101	X	-	-	-
46	RRX	h1	101	X	-	-	-
47	CHL	G	601	X	-	-	-
47	CHL	G	605	X	-	-	-
47	CHL	G	606	X	-	-	-
47	CHL	G	607	X	-	-	-
47	CHL	G	608	X	-	-	-
47	CHL	G	609	X	-	-	-
47	CHL	G1	601	X	-	-	-
47	CHL	G1	605	X	-	-	-
47	CHL	G1	606	X	-	-	-
47	CHL	G1	607	X	-	-	-
47	CHL	G1	608	X	-	-	-
47	CHL	G1	609	X	-	-	-
47	CHL	N	601	X	-	-	-
47	CHL	N	605	X	-	-	-
47	CHL	N	606	X	-	-	-
47	CHL	N	607	X	-	-	-
47	CHL	N	608	X	-	-	-
47	CHL	N	609	X	-	-	-
47	CHL	N1	601	X	-	-	-
47	CHL	N1	605	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	N1	606	X	-	-	-
47	CHL	N1	607	X	-	-	-
47	CHL	N1	608	X	-	-	-
47	CHL	N1	609	X	-	-	-
47	CHL	R	606	X	-	-	-
47	CHL	R	607	X	-	-	-
47	CHL	R1	606	X	-	-	-
47	CHL	R1	607	X	-	-	-
47	CHL	S	601	X	-	-	-
47	CHL	S	606	X	-	-	-
47	CHL	S	607	X	-	-	-
47	CHL	S	608	X	-	-	-
47	CHL	S1	601	X	-	-	-
47	CHL	S1	606	X	-	-	-
47	CHL	S1	607	X	-	-	-
47	CHL	S1	608	X	-	-	-
47	CHL	Y	601	X	-	-	-
47	CHL	Y	605	X	-	-	-
47	CHL	Y	606	X	-	-	-
47	CHL	Y	607	X	-	-	-
47	CHL	Y	609	X	-	-	-
47	CHL	Y1	601	X	-	-	-
47	CHL	Y1	605	X	-	-	-
47	CHL	Y1	606	X	-	-	-
47	CHL	Y1	607	X	-	-	-
47	CHL	Y1	609	X	-	-	-
47	CHL	g	601	X	-	-	-
47	CHL	g	605	X	-	-	-
47	CHL	g	606	X	-	-	-
47	CHL	g	607	X	-	-	-
47	CHL	g	608	X	-	-	-
47	CHL	g	609	X	-	-	-
47	CHL	g1	601	X	-	-	-
47	CHL	g1	605	X	-	-	-
47	CHL	g1	606	X	-	-	-
47	CHL	g1	607	X	-	-	-
47	CHL	g1	608	X	-	-	-
47	CHL	g1	609	X	-	-	-
47	CHL	n	601	X	-	-	-
47	CHL	n	605	X	-	-	-
47	CHL	n	606	X	-	-	-
47	CHL	n	607	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	n	608	X	-	-	-
47	CHL	n	609	X	-	-	-
47	CHL	n1	601	X	-	-	-
47	CHL	n1	605	X	-	-	-
47	CHL	n1	606	X	-	-	-
47	CHL	n1	607	X	-	-	-
47	CHL	n1	608	X	-	-	-
47	CHL	n1	609	X	-	-	-
47	CHL	r	606	X	-	-	-
47	CHL	r	607	X	-	-	-
47	CHL	r1	606	X	-	-	-
47	CHL	r1	607	X	-	-	-
47	CHL	s	601	X	-	-	-
47	CHL	s	606	X	-	-	-
47	CHL	s	607	X	-	-	-
47	CHL	s	608	X	-	-	-
47	CHL	s1	601	X	-	-	-
47	CHL	s1	606	X	-	-	-
47	CHL	s1	607	X	-	-	-
47	CHL	s1	608	X	-	-	-
47	CHL	y	601	X	-	-	-
47	CHL	y	605	X	-	-	-
47	CHL	y	606	X	-	-	-
47	CHL	y	607	X	-	-	-
47	CHL	y	609	X	-	-	-
47	CHL	y1	601	X	-	-	-
47	CHL	y1	605	X	-	-	-
47	CHL	y1	606	X	-	-	-
47	CHL	y1	607	X	-	-	-
47	CHL	y1	609	X	-	-	-
48	LUT	G	621	X	-	-	-
48	LUT	R1	620	X	-	-	-
48	LUT	S	620	X	-	-	-
48	LUT	Y	621	X	-	-	-
48	LUT	g1	621	X	-	-	-
48	LUT	n	621	X	-	-	-
48	LUT	s	620	X	-	-	-
49	XAT	G	622	X	-	-	-
49	XAT	G1	622	X	-	-	-
49	XAT	N	622	X	-	-	-
49	XAT	N1	622	X	-	-	-
49	XAT	R	621	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
49	XAT	Y	622	X	-	-	-
49	XAT	Y1	622	X	-	-	-
49	XAT	g	622	X	-	-	-
49	XAT	g1	622	X	-	-	-
49	XAT	n1	622	X	-	-	-
49	XAT	r	622	X	-	-	-
49	XAT	r1	621	X	-	-	-
56	ERG	R1	626	X	-	-	-
56	ERG	r1	626	X	-	-	-

## 2 Entry composition i

There are 57 unique types of molecules in this entry. The entry contains 151508 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	336	2638	1721	432	468	17	1	0
1	a	336	2638	1721	432	468	17	1	0
1	A1	336	2638	1721	432	468	17	1	0
1	a1	336	2638	1721	432	468	17	1	0

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	484	3783	2480	630	663	10	0	0
2	b	484	3783	2480	630	663	10	0	0
2	B1	484	3783	2480	630	663	10	0	0
2	b1	484	3783	2480	630	663	10	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	VAL	LEU	variant	UNP D0FY05
B	415	SER	LEU	variant	UNP D0FY05
b	298	VAL	LEU	variant	UNP D0FY05
b	415	SER	LEU	variant	UNP D0FY05
B1	298	VAL	LEU	variant	UNP D0FY05
B1	415	SER	LEU	variant	UNP D0FY05
b1	298	VAL	LEU	variant	UNP D0FY05
b1	415	SER	LEU	variant	UNP D0FY05

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		
3	V1	32	Total	C	N	O	0	0
			227	152	37	38		
3	v1	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	C1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c1	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	D1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d1	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	319	ILE	LEU	variant	UNP D0FXW8
d	319	ILE	LEU	variant	UNP D0FXW8
D1	319	ILE	LEU	variant	UNP D0FXW8
d1	319	ILE	LEU	variant	UNP D0FXW8

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		
6	E1	76	Total	C	N	O	0	0
			621	404	102	115		
6	e1	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	F1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f1	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	H1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h1	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	85	ALA	SER	variant	UNP D0FY02
h	85	ALA	SER	variant	UNP D0FY02
H1	85	ALA	SER	variant	UNP D0FY02
h1	85	ALA	SER	variant	UNP D0FY02

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		
10	j	36	Total	C	N	O	0	0
			266	183	40	43		
10	J1	36	Total	C	N	O	0	0
			266	183	40	43		
10	j1	36	Total	C	N	O	0	0
			266	183	40	43		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	variant	UNP D0FXW2
J	28	ALA	GLY	variant	UNP D0FXW2
J	42	LEU	GLN	variant	UNP D0FXW2
j	7	ILE	THR	variant	UNP D0FXW2
j	28	ALA	GLY	variant	UNP D0FXW2
j	42	LEU	GLN	variant	UNP D0FXW2
J1	7	ILE	THR	variant	UNP D0FXW2
J1	28	ALA	GLY	variant	UNP D0FXW2
J1	42	LEU	GLN	variant	UNP D0FXW2
j1	7	ILE	THR	variant	UNP D0FXW2
j1	28	ALA	GLY	variant	UNP D0FXW2
j1	42	LEU	GLN	variant	UNP D0FXW2

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	L1	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total	C	N	O	0	0
			243	164	34	45		
13	m	32	Total	C	N	O	0	0
			243	164	34	45		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	variant	UNP D0FXZ3
m	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	O1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o1	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	x1	30	201	132	32	37	0	0

- Molecule 19 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	61	457	312	68	76	1	0	0
19	z	61	457	312	68	76	1	0	0
19	Z1	61	457	312	68	76	1	0	0
19	z1	61	457	312	68	76	1	0	0

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	N	222	1703	1100	277	321	5	0	0
20	n	222	1703	1100	277	321	5	0	0
20	N1	222	1703	1100	277	321	5	0	0
20	n1	222	1703	1100	277	321	5	0	0

- Molecule 21 is a protein called LHCII M2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	221	1680	1085	271	321	3	0	0
21	g	221	1680	1085	271	321	3	0	0
21	G1	221	1680	1085	271	321	3	0	0
21	g1	221	1680	1085	271	321	3	0	0

- Molecule 22 is a protein called CP29.



Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		
22	r	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	242	Total	C	N	O	S	0	0
			1849	1195	297	354	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	U1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	M1	31	Total	C	N	O	0	0
			234	159	33	42		
26	m1	31	Total	C	N	O	0	0
			234	159	33	42		

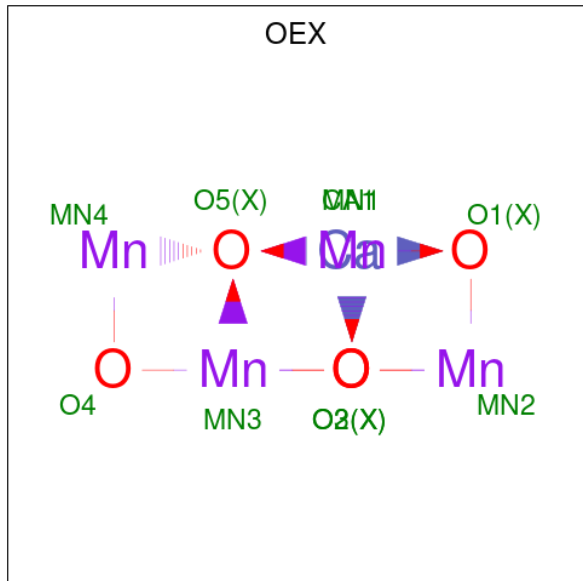
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	9	THR	ILE	variant	UNP D0FXZ3
m1	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 27 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	R1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		
27	r1	196	Total	C	N	O	P	S	0	0
			1490	943	251	292	1	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
28	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
28	A1	1	10	1	4	5	0
28	a1	1	10	1	4	5	0

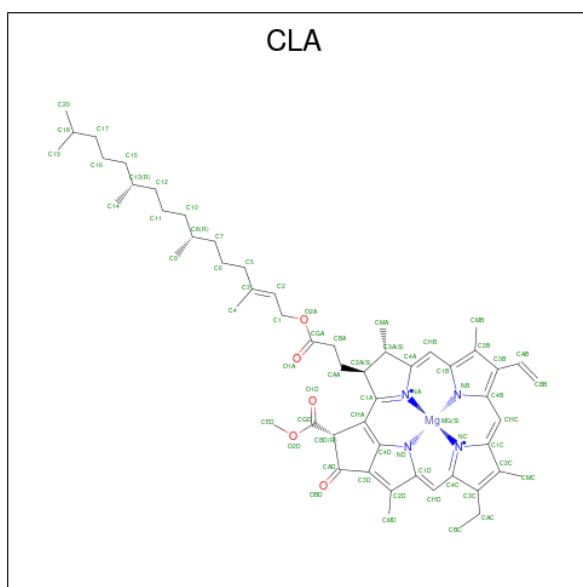
- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Fe	0
			1	1	
29	a	1	Total	Fe	0
			1	1	
29	A1	1	Total	Fe	0
			1	1	
29	a1	1	Total	Fe	0
			1	1	

- Molecule 30 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	Cl	0
			2	2	
30	a	2	Total	Cl	0
			2	2	
30	A1	2	Total	Cl	0
			2	2	
30	a1	2	Total	Cl	0
			2	2	

- Molecule 31 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	D	1	65	55	1	4	5	0
31	D	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	R	1	60	50	1	4	5	0
31	R	1	46	36	1	4	5	0
31	R	1	60	50	1	4	5	0
31	R	1	46	36	1	4	5	0
31	S	1	60	50	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	55	45	1	4	5	0
31	S	1	50	40	1	4	5	0
31	S	1	60	50	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	45	35	1	4	5	0
31	S	1	55	45	1	4	5	0
31	S	1	55	45	1	4	5	0
31	S	1	50	40	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	50	40	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	a	1	65	55	1	4	5	0
31	a	1	65	55	1	4	5	0
31	a	1	49	39	1	4	5	0
31	a	1	60	50	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	d	1	65	55	1	4	5	0
31	d	1	65	55	1	4	5	0
31	n	1	65	55	1	4	5	0
31	n	1	65	55	1	4	5	0
31	n	1	65	55	1	4	5	0
31	n	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
31	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	s	1	60	50	1	4	5	0
31	s	1	65	55	1	4	5	0
31	s	1	55	45	1	4	5	0
31	s	1	50	40	1	4	5	0
31	s	1	60	50	1	4	5	0
31	s	1	65	55	1	4	5	0
31	s	1	65	55	1	4	5	0
31	s	1	45	35	1	4	5	0
31	s	1	55	45	1	4	5	0
31	s	1	55	45	1	4	5	0
31	s	1	50	40	1	4	5	0
31	y	1	65	55	1	4	5	0
31	y	1	65	55	1	4	5	0
31	y	1	65	55	1	4	5	0
31	y	1	50	40	1	4	5	0
31	y	1	65	55	1	4	5	0
31	y	1	65	55	1	4	5	0
31	y	1	65	55	1	4	5	0
31	y	1	65	55	1	4	5	0
31	A1	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
31	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	C1	1	65	55	1	4	5	0
31	D1	1	65	55	1	4	5	0
31	D1	1	65	55	1	4	5	0
31	N1	1	65	55	1	4	5	0
31	N1	1	65	55	1	4	5	0
31	N1	1	65	55	1	4	5	0
31	N1	1	65	55	1	4	5	0
31	N1	1	49	39	1	4	5	0
31	N1	1	45	35	1	4	5	0
31	N1	1	65	55	1	4	5	0
31	N1	1	49	39	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	S1	1	65	55	1	4	5	0
31	S1	1	45	35	1	4	5	0
31	S1	1	55	45	1	4	5	0
31	S1	1	55	45	1	4	5	0
31	S1	1	50	40	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	50	40	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	Y1	1	65	55	1	4	5	0
31	a1	1	65	55	1	4	5	0
31	a1	1	65	55	1	4	5	0
31	a1	1	49	39	1	4	5	0
31	a1	1	60	50	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	b1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0
31	c1	1	65	55	1	4	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

*Continued on next page...*

*Continued from previous page...*

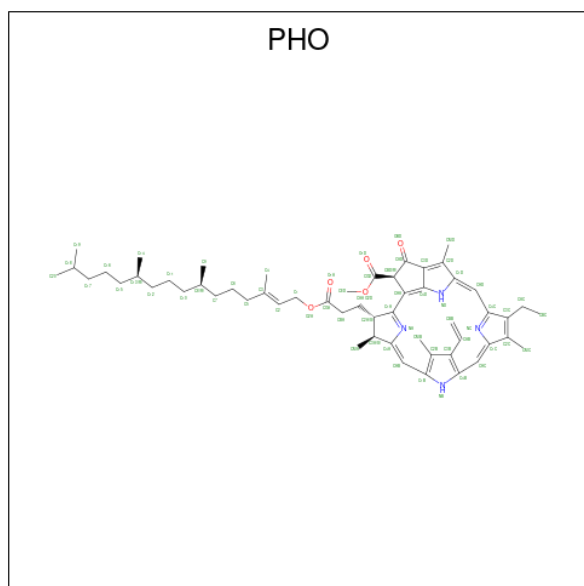
Mol	Chain	Residues	Atoms					AltConf
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



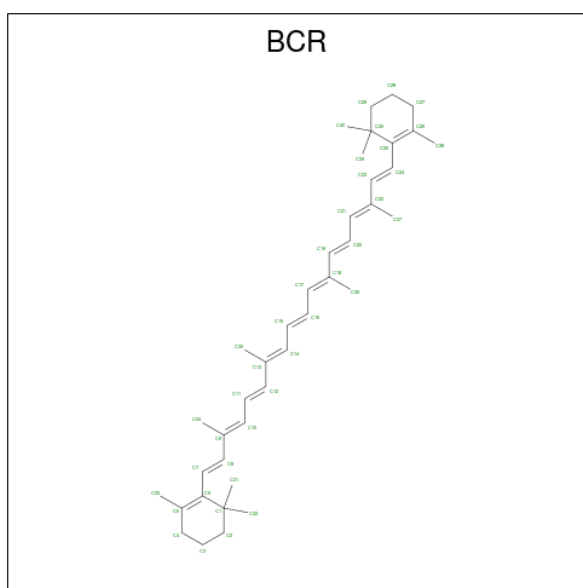
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	N	O	0
			64	55	4	5	
32	A	1	Total	C	N	O	0
			64	55	4	5	
32	a	1	Total	C	N	O	0
			64	55	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
32	a	1	Total 64	C 55	N 4	O 5	0
32	A1	1	Total 64	C 55	N 4	O 5	0
32	A1	1	Total 64	C 55	N 4	O 5	0
32	a1	1	Total 64	C 55	N 4	O 5	0
32	a1	1	Total 64	C 55	N 4	O 5	0

- Molecule 33 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total 40	C 40	0
33	B	1	Total 40	C 40	0
33	B	1	Total 40	C 40	0
33	C	1	Total 40	C 40	0
33	C	1	Total 40	C 40	0
33	C	1	Total 40	C 40	0

Continued on next page...

*Continued from previous page...*

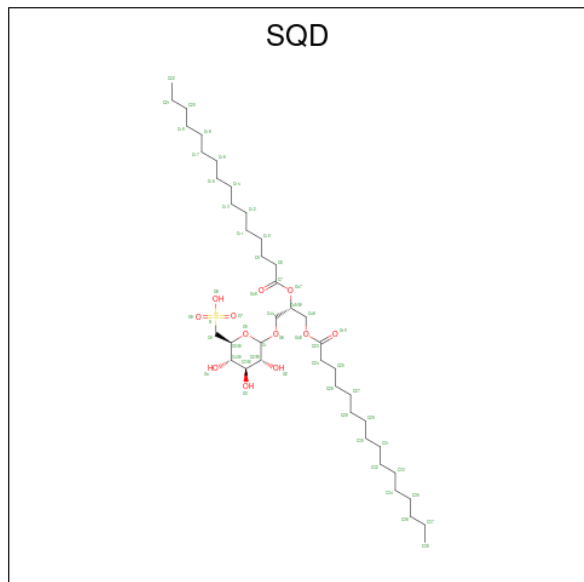
Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total C 40 40	0
33	D	1	Total C 40 40	0
33	a	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	d	1	Total C 40 40	0
33	A1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	D1	1	Total C 40 40	0
33	a1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
33	c1	1	Total C 40 40	0
33	c1	1	Total C 40 40	0
33	c1	1	Total C 40 40	0
33	c1	1	Total C 40 40	0
33	d1	1	Total C 40 40	0

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



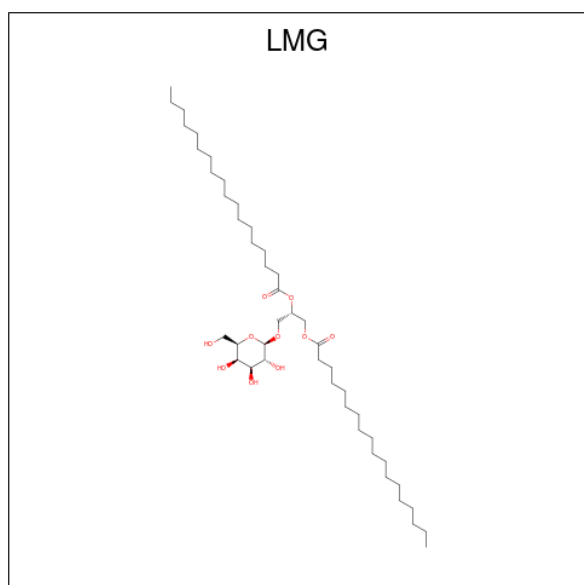
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C O S 51 38 12 1	0
34	B	1	Total C O S 54 41 12 1	0
34	C	1	Total C O S 54 41 12 1	0
34	a	1	Total C O S 51 38 12 1	0
34	b	1	Total C O S 54 41 12 1	0
34	c	1	Total C O S 54 41 12 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
34	A1	1	Total 51	C 38	O 12	S 1	0
34	B1	1	Total 42	C 29	O 12	S 1	0
34	B1	1	Total 54	C 41	O 12	S 1	0
34	C1	1	Total 54	C 41	O 12	S 1	0
34	M1	1	Total 42	C 29	O 12	S 1	0
34	a1	1	Total 51	C 38	O 12	S 1	0
34	b1	1	Total 42	C 29	O 12	S 1	0
34	b1	1	Total 54	C 41	O 12	S 1	0
34	c1	1	Total 54	C 41	O 12	S 1	0
34	m1	1	Total 42	C 29	O 12	S 1	0

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	A	1	Total 48	C 38	O 10	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	B	1	44	34	10	0
35	C	1	51	41	10	0
35	D	1	46	36	10	0
35	H	1	48	38	10	0
35	J	1	45	35	10	0
35	a	1	48	38	10	0
35	b	1	44	34	10	0
35	c	1	51	41	10	0
35	d	1	46	36	10	0
35	h	1	48	38	10	0
35	j	1	45	35	10	0
35	A1	1	48	38	10	0
35	B1	1	44	34	10	0
35	C1	1	51	41	10	0
35	C1	1	55	45	10	0
35	D1	1	46	36	10	0
35	H1	1	48	38	10	0
35	W1	1	39	29	10	0
35	a1	1	48	38	10	0
35	b1	1	44	34	10	0
35	c1	1	51	41	10	0

*Continued on next page...*



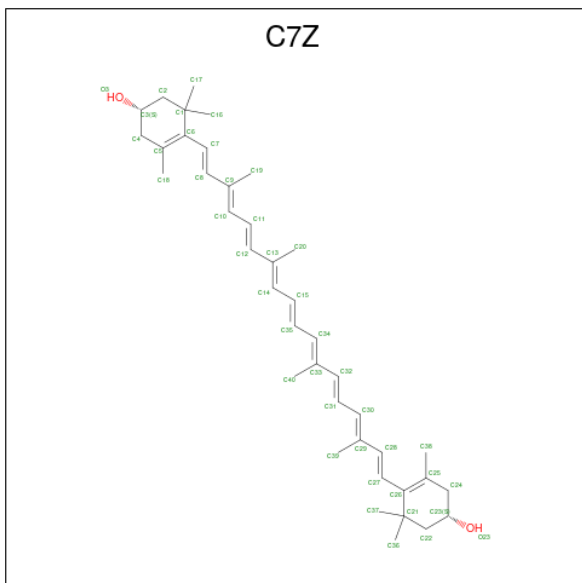
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
35	c1	1	Total	C	O	0
			55	45	10	
35	d1	1	Total	C	O	0
			46	36	10	
35	h1	1	Total	C	O	0
			48	38	10	
35	w1	1	Total	C	O	0
			39	29	10	

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

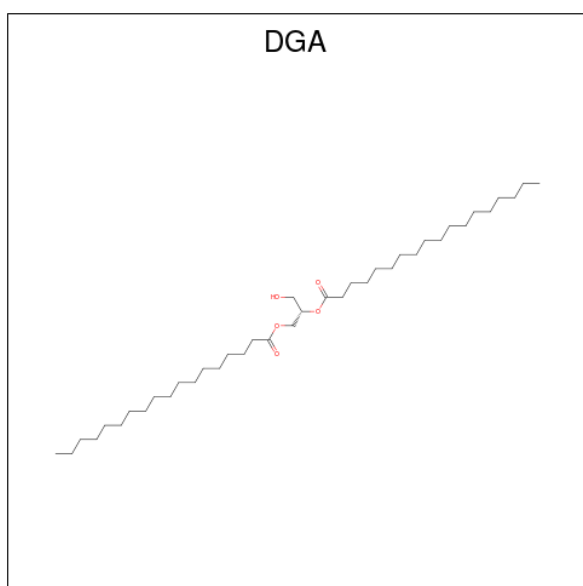
Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Na	0
			1	1	
36	a	1	Total	Na	0
			1	1	
36	A1	1	Total	Na	0
			1	1	
36	a1	1	Total	Na	0
			1	1	

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]oc tadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			42	40	2	
37	b	1	Total	C	O	0
			42	40	2	
37	B1	1	Total	C	O	0
			42	40	2	
37	b1	1	Total	C	O	0
			42	40	2	

- Molecule 38 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



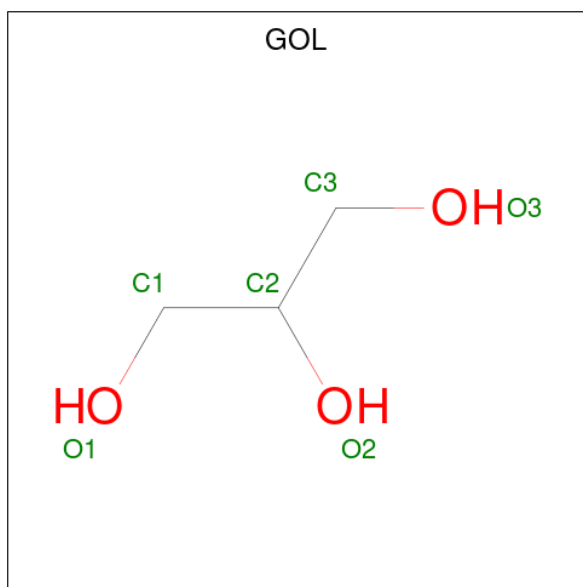
Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			44	39	5	
38	C	1	Total	C	O	0
			44	39	5	
38	b	1	Total	C	O	0
			44	39	5	
38	c	1	Total	C	O	0
			44	39	5	
38	B1	1	Total	C	O	0
			44	39	5	
38	C1	1	Total	C	O	0
			44	39	5	
38	J1	1	Total	C	O	0
			29	24	5	
38	b1	1	Total	C	O	0
			44	39	5	

*Continued on next page...*

Continued from previous page...

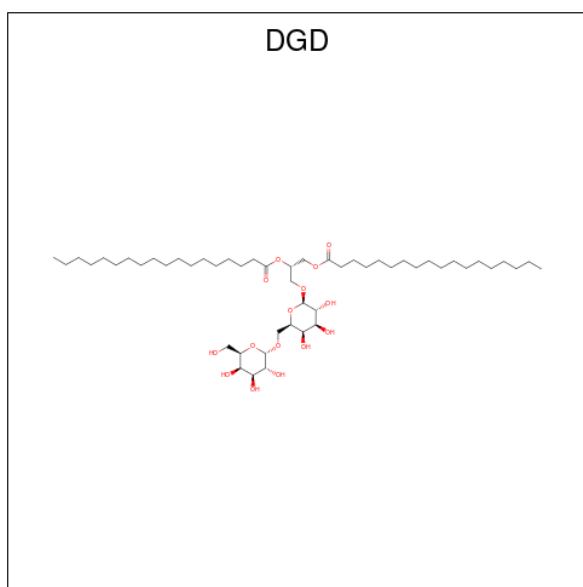
Mol	Chain	Residues	Atoms			AltConf
38	c1	1	Total	C	O	0
			44	39	5	
38	j1	1	Total	C	O	0
			29	24	5	

- Molecule 39 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			6	3	3	
39	b	1	Total	C	O	0
			6	3	3	
39	b	1	Total	C	O	0
			6	3	3	
39	y	1	Total	C	O	0
			6	3	3	
39	I1	1	Total	C	O	0
			6	3	3	

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



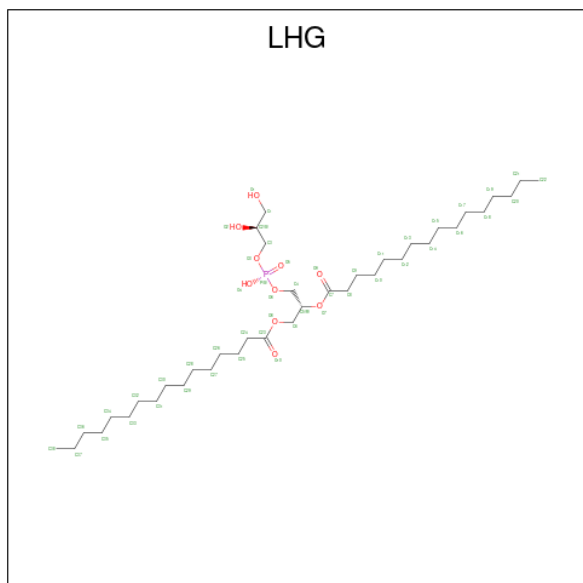
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	C	1	55	40	15	0
40	C	1	62	47	15	0
40	C	1	59	44	15	0
40	C	1	66	51	15	0
40	c	1	55	40	15	0
40	c	1	62	47	15	0
40	c	1	59	44	15	0
40	c	1	66	51	15	0
40	B1	1	43	28	15	0
40	C1	1	55	40	15	0
40	C1	1	62	47	15	0
40	C1	1	59	44	15	0
40	b1	1	43	28	15	0
40	c1	1	55	40	15	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	c1	1	62	47	15	0
40	c1	1	59	44	15	0

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	C	1	47	36	10	1	0
41	D	1	44	33	10	1	0
41	D	1	49	38	10	1	0
41	D	1	39	28	10	1	0
41	L	1	49	38	10	1	0
41	N	1	49	38	10	1	0
41	G	1	49	38	10	1	0
41	S	1	45	34	10	1	0
41	Y	1	49	38	10	1	0

Continued on next page...

*Continued from previous page...*

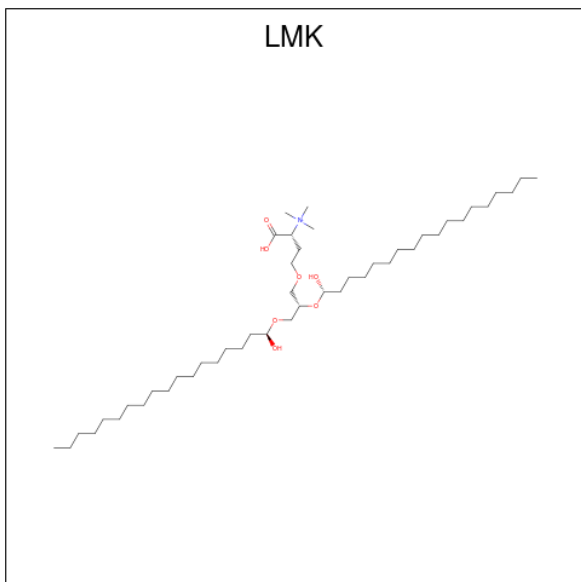
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	c	1	47	36	10	1	0
41	d	1	44	33	10	1	0
41	d	1	49	38	10	1	0
41	d	1	39	28	10	1	0
41	l	1	49	38	10	1	0
41	n	1	49	38	10	1	0
41	g	1	49	38	10	1	0
41	s	1	45	34	10	1	0
41	y	1	49	38	10	1	0
41	C1	1	47	36	10	1	0
41	D1	1	44	33	10	1	0
41	D1	1	49	38	10	1	0
41	D1	1	39	28	10	1	0
41	L1	1	49	38	10	1	0
41	N1	1	49	38	10	1	0
41	G1	1	49	38	10	1	0
41	S1	1	45	34	10	1	0
41	Y1	1	49	38	10	1	0
41	c1	1	47	36	10	1	0
41	d1	1	44	33	10	1	0
41	d1	1	49	38	10	1	0

*Continued on next page...*

Continued from previous page...

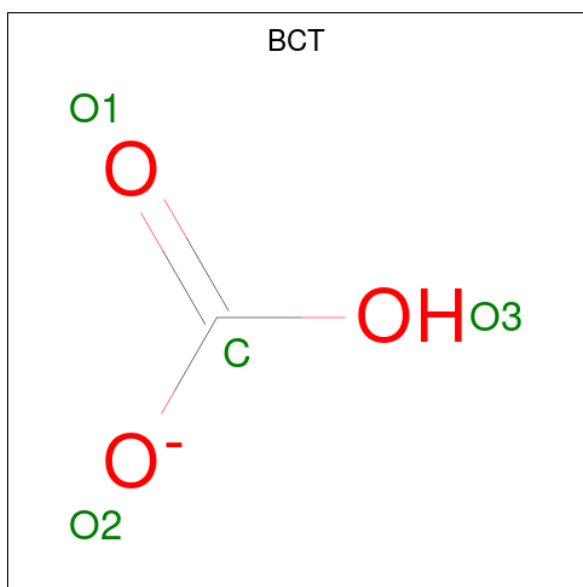
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	d1	1	Total 39	C 28	O 10	P 1	0
41	n1	1	Total 49	C 38	O 10	P 1	0
41	g1	1	Total 49	C 38	O 10	P 1	0
41	s1	1	Total 45	C 34	O 10	P 1	0
41	y1	1	Total 49	C 38	O 10	P 1	0

- Molecule 42 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxido-nyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (three-letter code: LMK) (formula: C<sub>46</sub>H<sub>94</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
42	C	1	Total 40	C 32	N 1	O 7	0
42	c	1	Total 40	C 32	N 1	O 7	0
42	C1	1	Total 40	C 32	N 1	O 7	0
42	c1	1	Total 40	C 32	N 1	O 7	0

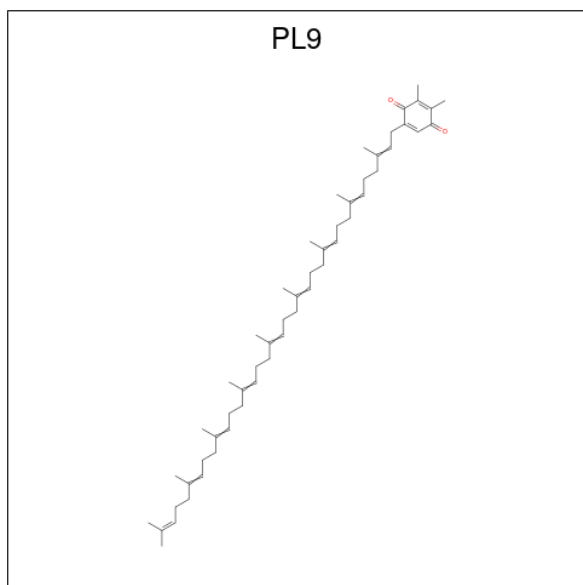
- Molecule 43 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
43	D	1	4	1	3	0
43	d	1	4	1	3	0
43	D1	1	4	1	3	0
43	d1	1	4	1	3	0

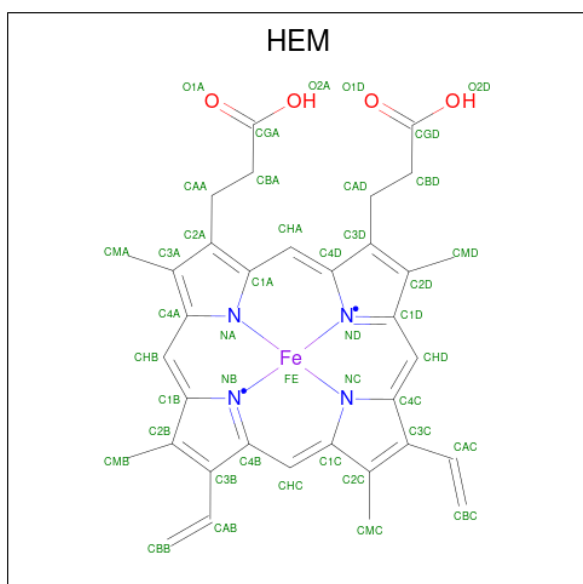
- Molecule 44 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).





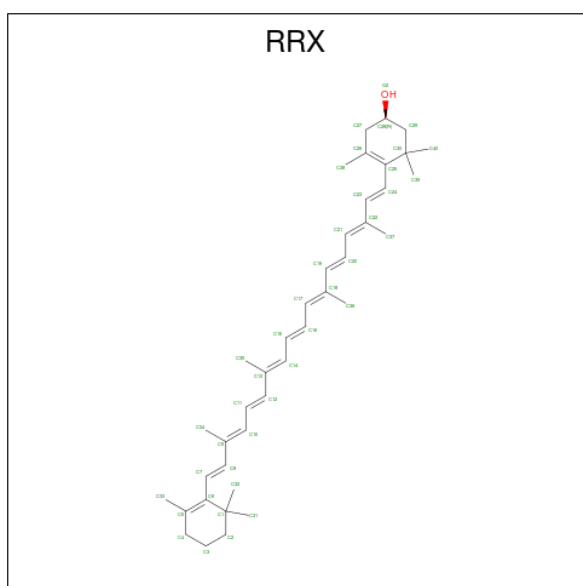
Mol	Chain	Residues	Atoms			AltConf
44	D	1	Total	C	O	0
			55	53	2	
44	d	1	Total	C	O	0
			55	53	2	
44	D1	1	Total	C	O	0
			55	53	2	
44	d1	1	Total	C	O	0
			55	53	2	

- Molecule 45 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



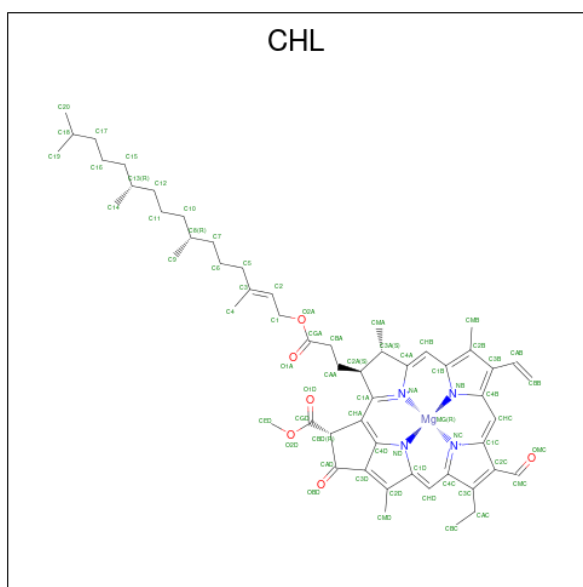
Mol	Chain	Residues	Atoms				AltConf	
45	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	F1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 46 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms		AltConf
46	H	1	Total	C O	0
			41	40 1	
46	h	1	Total	C O	0
			41	40 1	
46	H1	1	Total	C O	0
			41	40 1	
46	h1	1	Total	C O	0
			41	40 1	

- Molecule 47 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
47	N	1	66	55	1	4	6	0
47	N	1	66	55	1	4	6	0
47	N	1	66	55	1	4	6	0
47	N	1	66	55	1	4	6	0
47	N	1	50	39	1	4	6	0
47	N	1	66	55	1	4	6	0
47	G	1	66	55	1	4	6	0
47	G	1	48	37	1	4	6	0
47	G	1	50	39	1	4	6	0
47	G	1	50	39	1	4	6	0
47	G	1	44	35	1	4	4	0
47	G	1	66	55	1	4	6	0
47	R	1	44	35	1	4	4	0
47	R	1	50	39	1	4	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
47	S	1	46	35	1	4	6	0
47	S	1	44	35	1	4	4	0
47	S	1	43	34	1	4	4	0
47	S	1	61	50	1	4	6	0
47	Y	1	66	55	1	4	6	0
47	Y	1	46	35	1	4	6	0
47	Y	1	66	55	1	4	6	0
47	Y	1	66	55	1	4	6	0
47	Y	1	66	55	1	4	6	0
47	n	1	66	55	1	4	6	0
47	n	1	66	55	1	4	6	0
47	n	1	66	55	1	4	6	0
47	n	1	66	55	1	4	6	0
47	n	1	50	39	1	4	6	0
47	n	1	66	55	1	4	6	0
47	g	1	66	55	1	4	6	0
47	g	1	48	37	1	4	6	0
47	g	1	50	39	1	4	6	0
47	g	1	50	39	1	4	6	0
47	g	1	44	35	1	4	4	0
47	g	1	66	55	1	4	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
			Total	C	Mg	N O	
47	r	1	44	35	1	4 4	0
47	r	1	50	39	1	4 6	0
47	s	1	46	35	1	4 6	0
47	s	1	44	35	1	4 4	0
47	s	1	43	34	1	4 4	0
47	s	1	61	50	1	4 6	0
47	y	1	66	55	1	4 6	0
47	y	1	46	35	1	4 6	0
47	y	1	66	55	1	4 6	0
47	y	1	66	55	1	4 6	0
47	y	1	66	55	1	4 6	0
47	N1	1	66	55	1	4 6	0
47	N1	1	66	55	1	4 6	0
47	N1	1	66	55	1	4 6	0
47	N1	1	66	55	1	4 6	0
47	N1	1	50	39	1	4 6	0
47	N1	1	66	55	1	4 6	0
47	G1	1	66	55	1	4 6	0
47	G1	1	48	37	1	4 6	0
47	G1	1	50	39	1	4 6	0
47	G1	1	66	55	1	4 6	0

*Continued on next page...*

*Continued from previous page...*

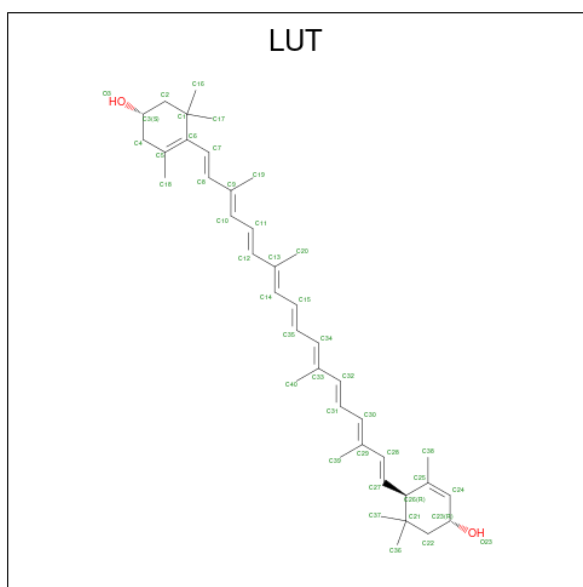
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
47	G1	1	44	35	1	4	4	0
47	G1	1	66	55	1	4	6	0
47	R1	1	44	35	1	4	4	0
47	R1	1	50	39	1	4	6	0
47	S1	1	46	35	1	4	6	0
47	S1	1	44	35	1	4	4	0
47	S1	1	43	34	1	4	4	0
47	S1	1	61	50	1	4	6	0
47	Y1	1	66	55	1	4	6	0
47	Y1	1	46	35	1	4	6	0
47	Y1	1	66	55	1	4	6	0
47	Y1	1	66	55	1	4	6	0
47	Y1	1	66	55	1	4	6	0
47	Y1	1	66	55	1	4	6	0
47	n1	1	66	55	1	4	6	0
47	n1	1	66	55	1	4	6	0
47	n1	1	66	55	1	4	6	0
47	n1	1	66	55	1	4	6	0
47	n1	1	50	39	1	4	6	0
47	n1	1	66	55	1	4	6	0
47	g1	1	66	55	1	4	6	0
47	g1	1	48	37	1	4	6	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
47	g1	1	50	39	1	4	6	0
47	g1	1	66	55	1	4	6	0
47	g1	1	44	35	1	4	4	0
47	g1	1	66	55	1	4	6	0
47	r1	1	44	35	1	4	4	0
47	r1	1	50	39	1	4	6	0
47	s1	1	46	35	1	4	6	0
47	s1	1	44	35	1	4	4	0
47	s1	1	43	34	1	4	4	0
47	s1	1	61	50	1	4	6	0
47	y1	1	66	55	1	4	6	0
47	y1	1	46	35	1	4	6	0
47	y1	1	66	55	1	4	6	0
47	y1	1	66	55	1	4	6	0
47	y1	1	66	55	1	4	6	0

- Molecule 48 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			42	40	2	
48	N	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	
48	R	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	r	1	Total	C	O	0
			42	40	2	

*Continued on next page...*



*Continued from previous page...*

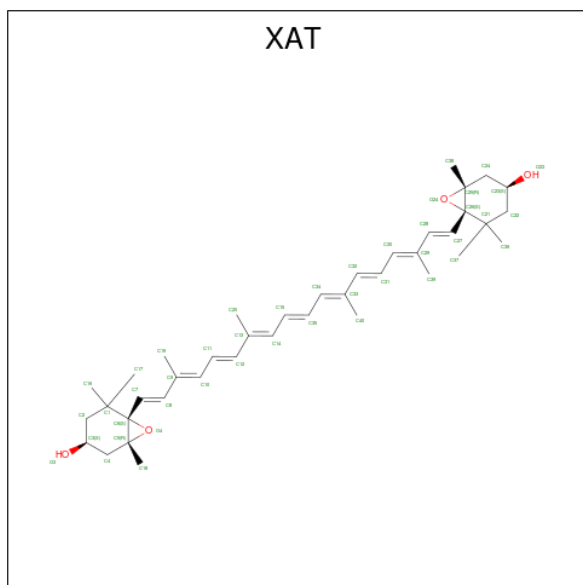
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	s	1	42	40	2	0
48	s	1	42	40	2	0
48	y	1	42	40	2	0
48	y	1	42	40	2	0
48	N1	1	42	40	2	0
48	N1	1	42	40	2	0
48	G1	1	42	40	2	0
48	G1	1	42	40	2	0
48	R1	1	42	40	2	0
48	S1	1	42	40	2	0
48	S1	1	42	40	2	0
48	Y1	1	42	40	2	0
48	Y1	1	42	40	2	0
48	n1	1	42	40	2	0
48	n1	1	42	40	2	0
48	g1	1	42	40	2	0
48	g1	1	42	40	2	0
48	r1	1	42	40	2	0
48	s1	1	42	40	2	0
48	s1	1	42	40	2	0
48	y1	1	42	40	2	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	y1	1	42	40	2	0

- Molecule 49 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



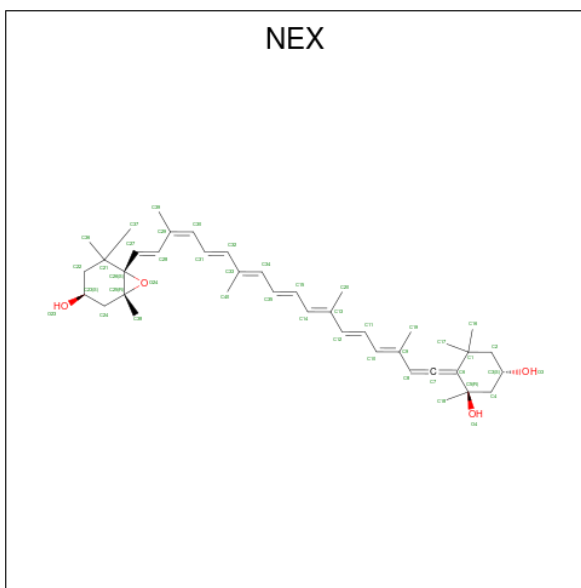
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
49	N	1	44	40	4	0
49	G	1	44	40	4	0
49	R	1	44	40	4	0
49	Y	1	44	40	4	0
49	n	1	44	40	4	0
49	g	1	44	40	4	0
49	r	1	44	40	4	0
49	y	1	44	40	4	0
49	N1	1	44	40	4	0
49	G1	1	44	40	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
49	R1	1	Total	C	O	0
			44	40	4	
49	Y1	1	Total	C	O	0
			44	40	4	
49	n1	1	Total	C	O	0
			44	40	4	
49	g1	1	Total	C	O	0
			44	40	4	
49	r1	1	Total	C	O	0
			44	40	4	
49	y1	1	Total	C	O	0
			44	40	4	

- Molecule 50 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



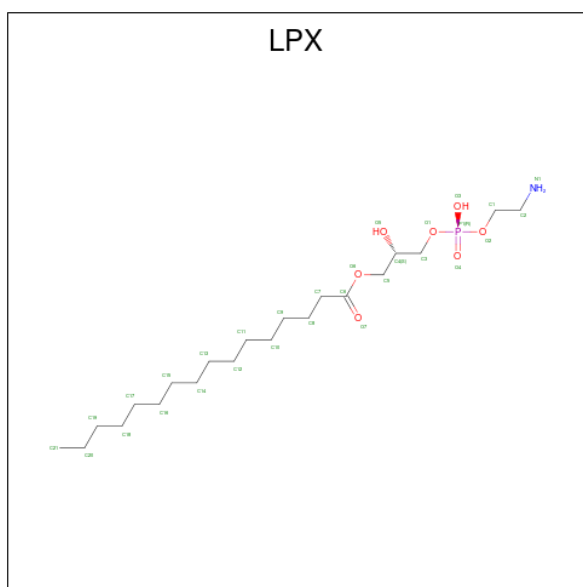
Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			44	40	4	
50	G	1	Total	C	O	0
			44	40	4	
50	R	1	Total	C	O	0
			44	40	4	
50	S	1	Total	C	O	0
			44	40	4	

Continued on next page...

Continued from previous page...

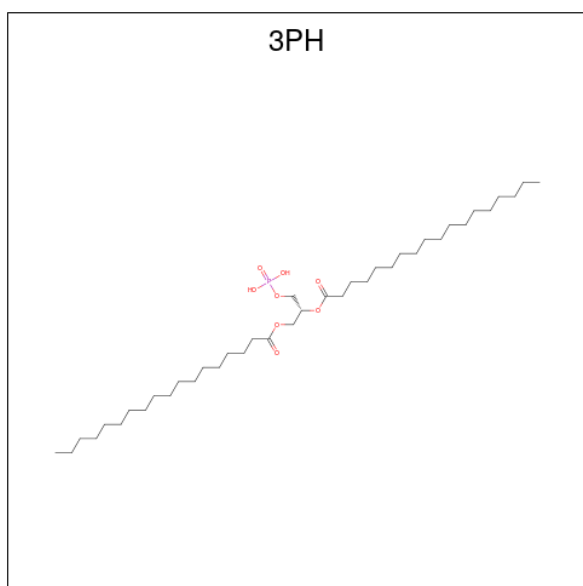
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	Y	1	44	40	4	0
50	n	1	44	40	4	0
50	g	1	44	40	4	0
50	r	1	44	40	4	0
50	s	1	44	40	4	0
50	y	1	44	40	4	0
50	N1	1	44	40	4	0
50	G1	1	44	40	4	0
50	R1	1	44	40	4	0
50	S1	1	44	40	4	0
50	Y1	1	44	40	4	0
50	n1	1	44	40	4	0
50	g1	1	44	40	4	0
50	r1	1	44	40	4	0
50	s1	1	44	40	4	0
50	y1	1	44	40	4	0

- Molecule 51 is (2S)-3-[[[R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C<sub>21</sub>H<sub>44</sub>NO<sub>7</sub>P).



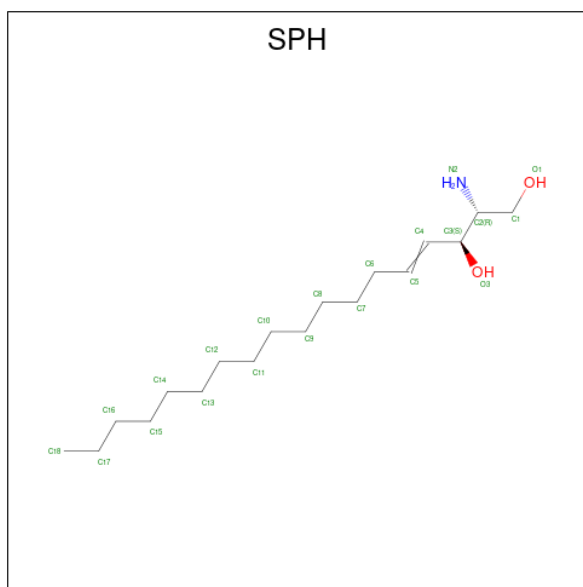
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	S	1	30	21	1	7	1	0
51	s	1	30	21	1	7	1	0
51	S1	1	30	21	1	7	1	0
51	s1	1	30	21	1	7	1	0

- Molecule 52 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				AltConf
52	S	1	Total	C	O	P	0
			48	39	8	1	
52	i	1	Total	C	O	P	0
			48	39	8	1	
52	s	1	Total	C	O	P	0
			48	39	8	1	
52	B1	1	Total	C	O	P	0
			48	39	8	1	
52	T1	1	Total	C	O	P	0
			48	39	8	1	
52	S1	1	Total	C	O	P	0
			48	39	8	1	
52	b1	1	Total	C	O	P	0
			48	39	8	1	
52	t1	1	Total	C	O	P	0
			48	39	8	1	
52	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 53 is SPHINGOSINE (three-letter code: SPH) (formula: C<sub>18</sub>H<sub>37</sub>NO<sub>2</sub>).



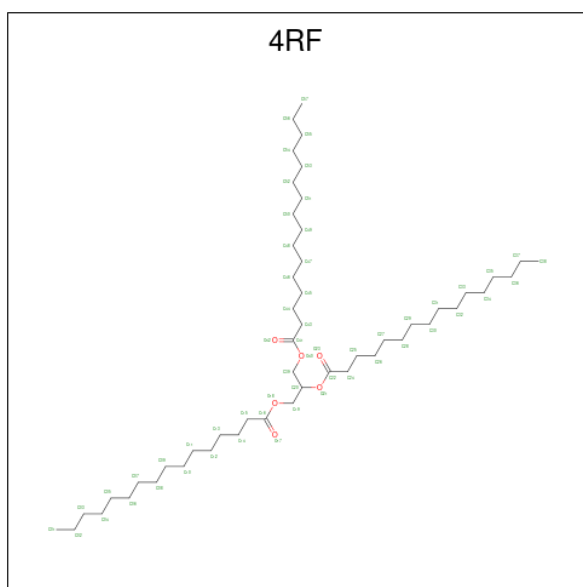
Mol	Chain	Residues	Atoms				AltConf
53	Y	1	Total	C	N	O	0
			21	18	1	2	
53	y	1	Total	C	N	O	0
			21	18	1	2	
53	A1	1	Total	C	N	O	0
			21	18	1	2	

*Continued on next page...*

Continued from previous page...

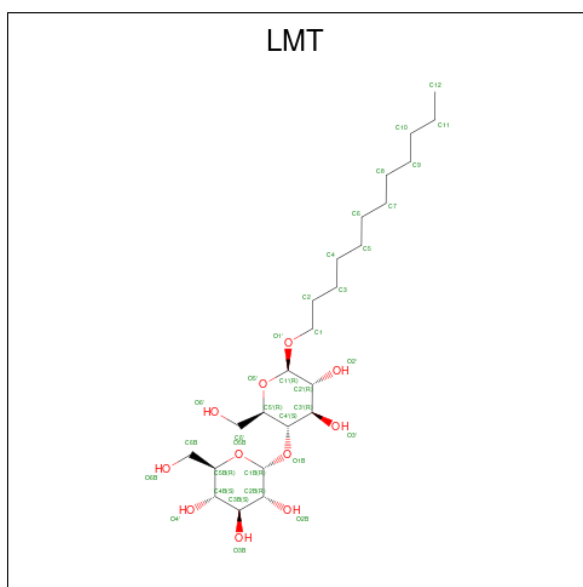
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
53	Y1	1	Total 21	C 18	N 1	O 2	0
53	a1	1	Total 21	C 18	N 1	O 2	0
53	y1	1	Total 21	C 18	N 1	O 2	0

- Molecule 54 is Tripalmitoylglycerol (three-letter code: 4RF) (formula:  $C_{51}H_{98}O_6$ ).



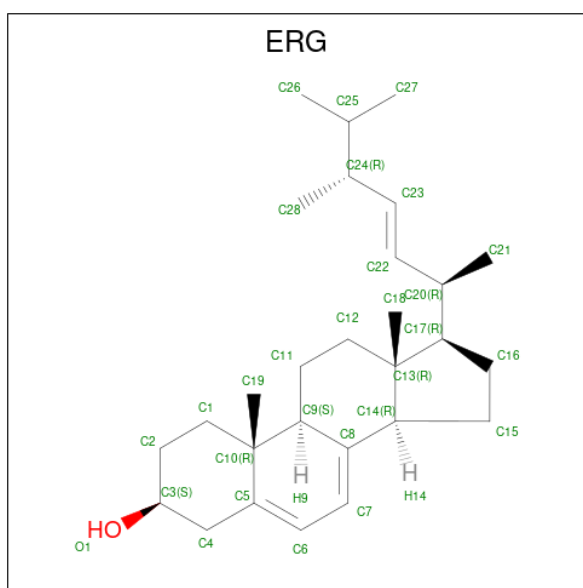
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
54	I1	1	Total 57	C 51	O 6	0
54	K1	1	Total 57	C 51	O 6	0
54	i1	1	Total 57	C 51	O 6	0
54	k1	1	Total 57	C 51	O 6	0

- Molecule 55 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
55	R1	1	Total	C	O	0
			35	24	11	
55	r1	1	Total	C	O	0
			35	24	11	

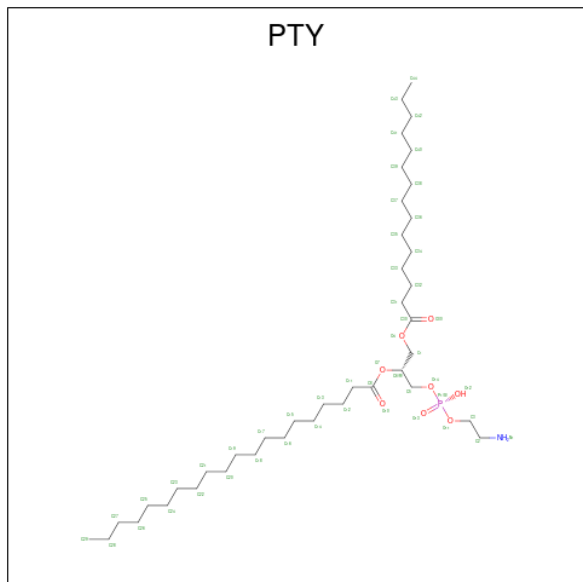
- Molecule 56 is ERGOSTEROL (three-letter code: ERG) (formula:  $C_{28}H_{44}O$ ).



Mol	Chain	Residues	Atoms			AltConf
56	R1	1	Total	C	O	0
			29	28	1	
56	r1	1	Total	C	O	0
			29	28	1	



- Molecule 57 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).

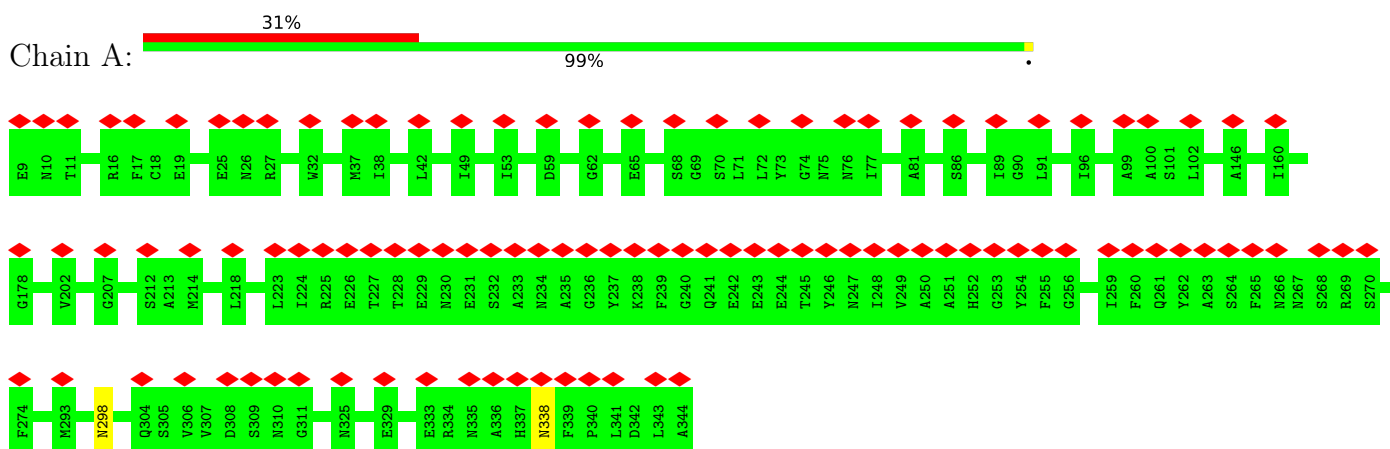


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	Y1	1	50	40	1	8	1	0
57	Y1	1	19	9	1	8	1	0
57	y1	1	50	40	1	8	1	0
57	y1	1	19	9	1	8	1	0

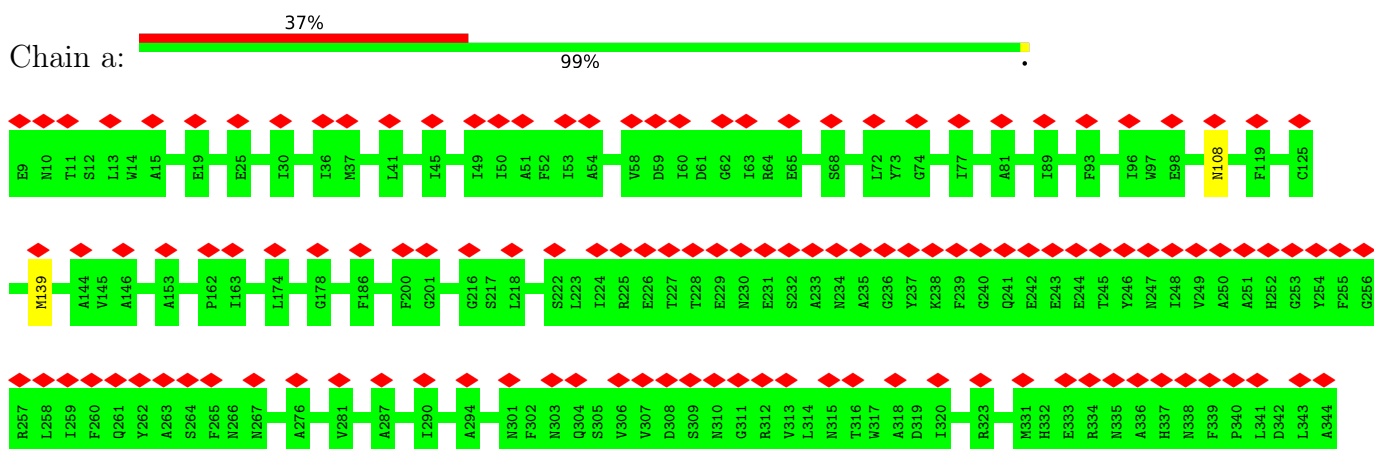
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

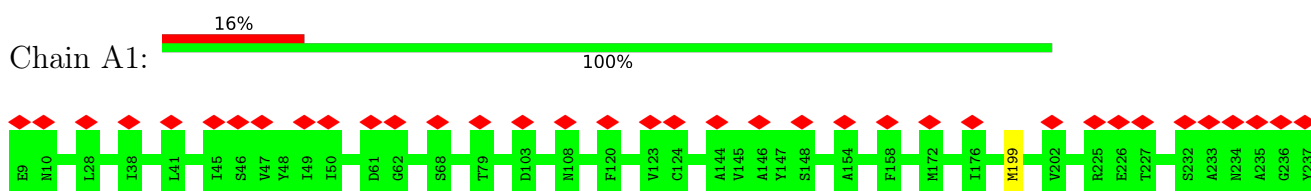
- Molecule 1: Photosystem II protein D1

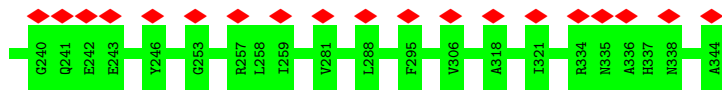


- Molecule 1: Photosystem II protein D1



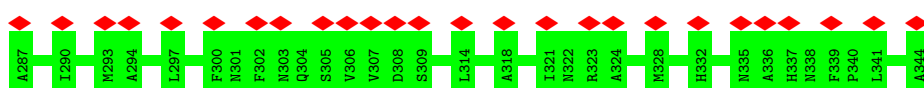
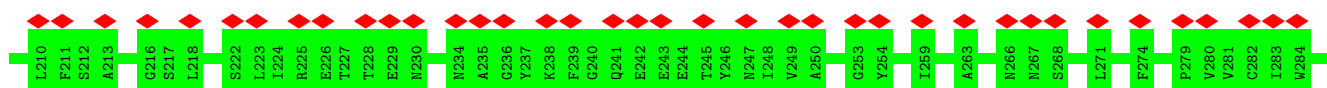
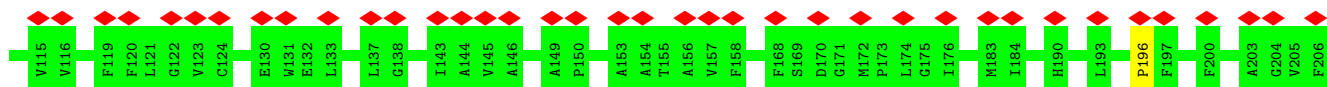
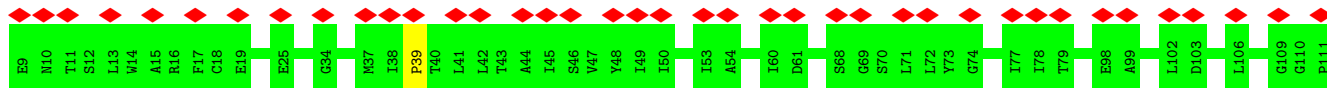
- Molecule 1: Photosystem II protein D1





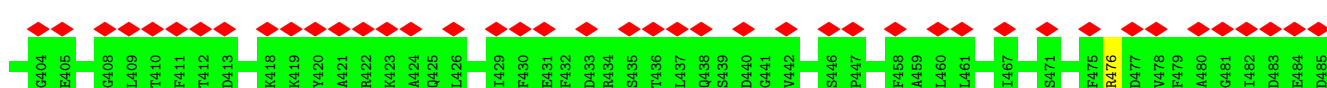
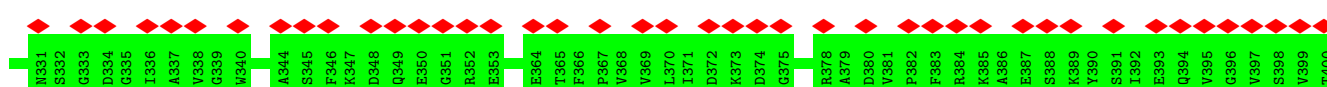
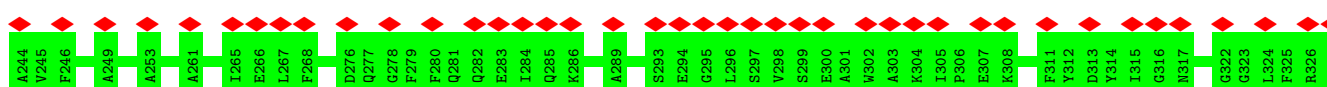
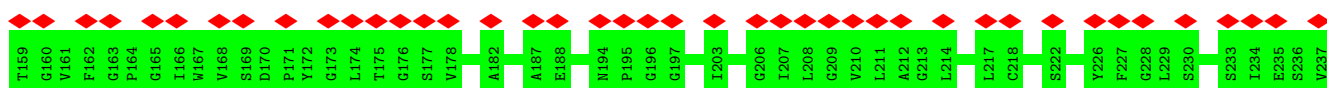
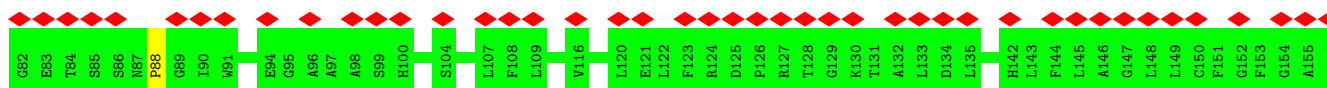
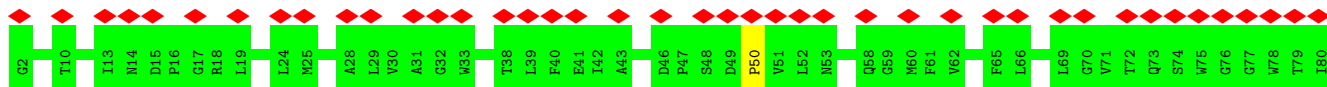
- Molecule 1: Photosystem II protein D1

Chain a1: 42% 99%

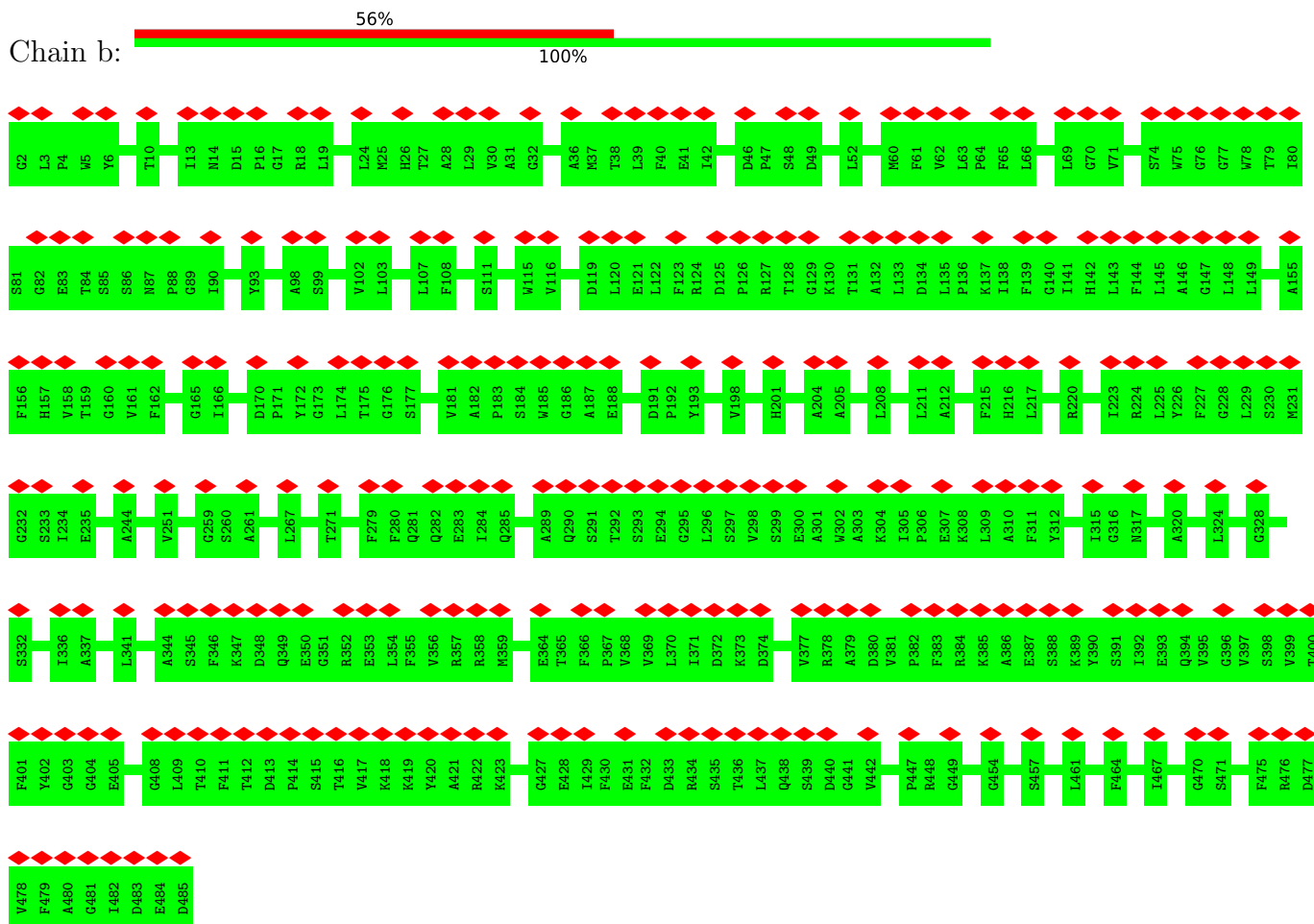


- Molecule 2: Photosystem II CP47 reaction center protein

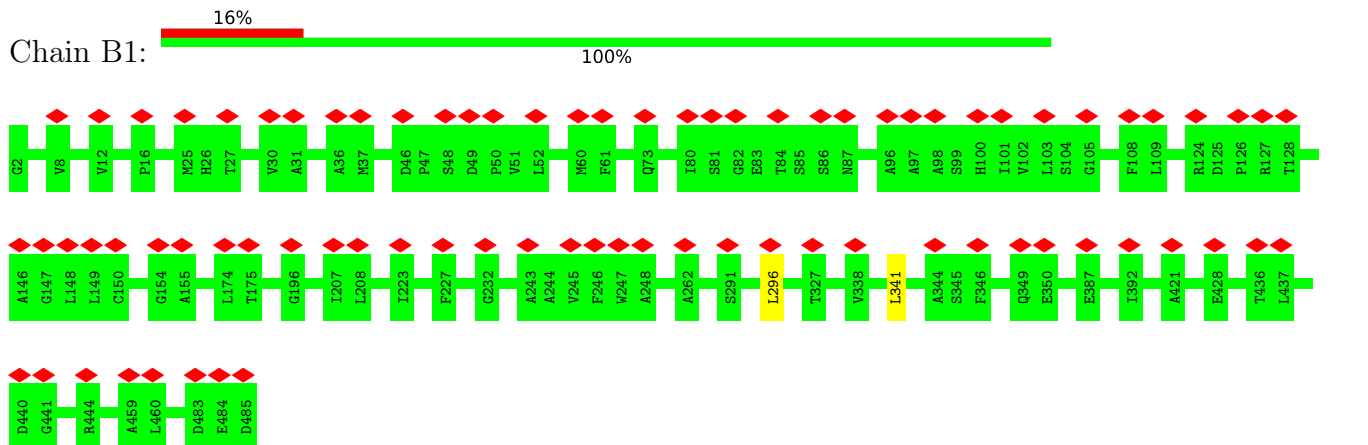
Chain B: 53% 99%



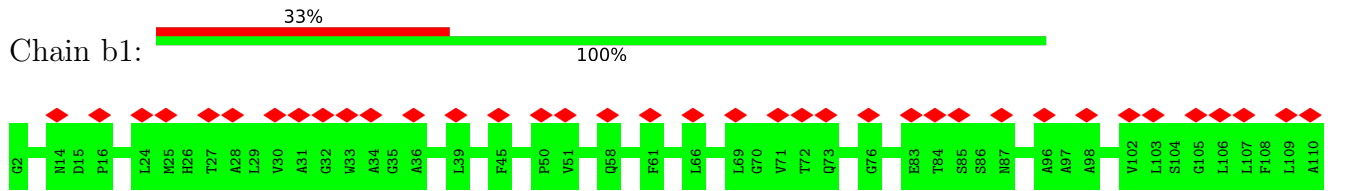
- Molecule 2: Photosystem II CP47 reaction center protein

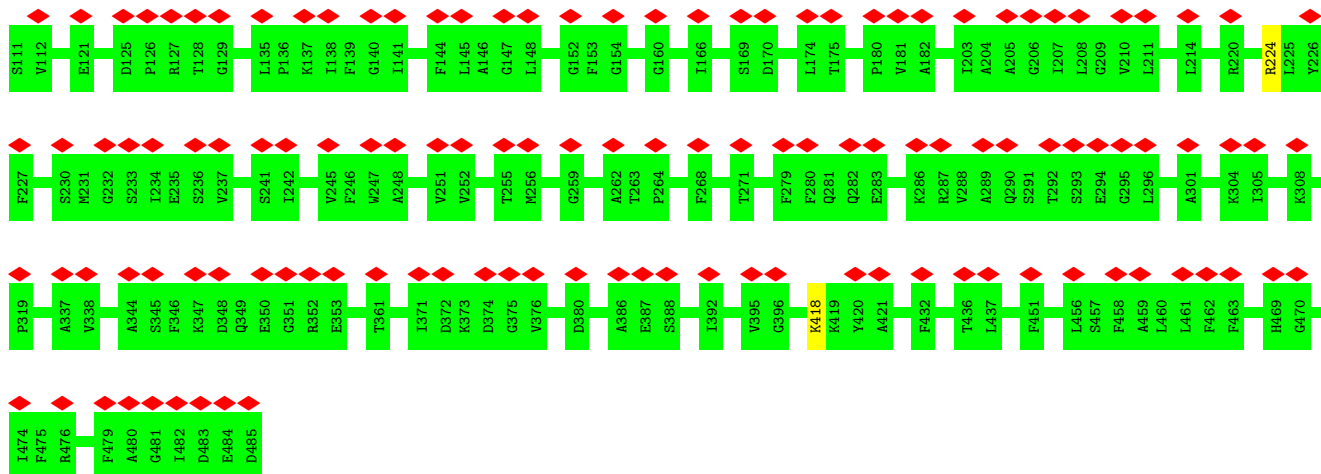


• Molecule 2: Photosystem II CP47 reaction center protein

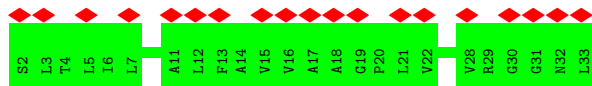


• Molecule 2: Photosystem II CP47 reaction center protein

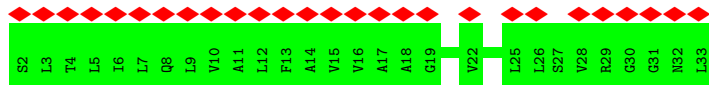
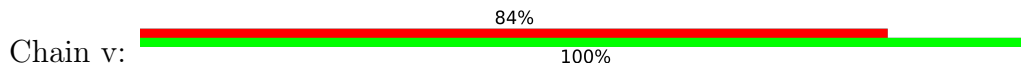




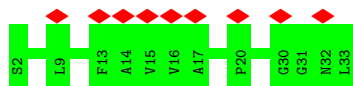
• Molecule 3: Photosystem II reaction center protein Ycf12



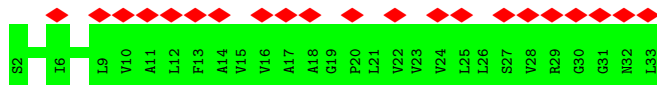
• Molecule 3: Photosystem II reaction center protein Ycf12



• Molecule 3: Photosystem II reaction center protein Ycf12

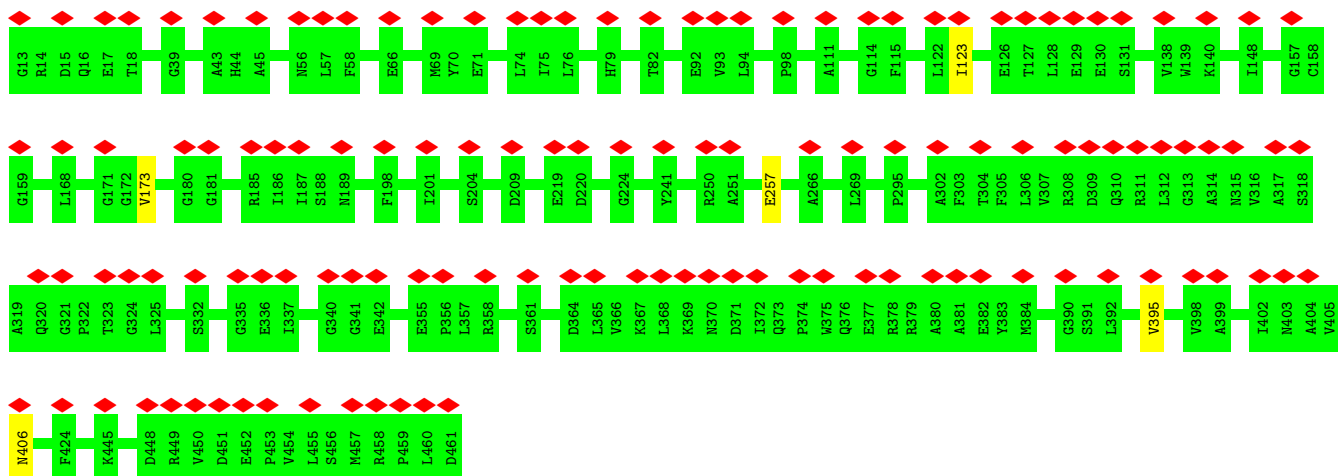


• Molecule 3: Photosystem II reaction center protein Ycf12

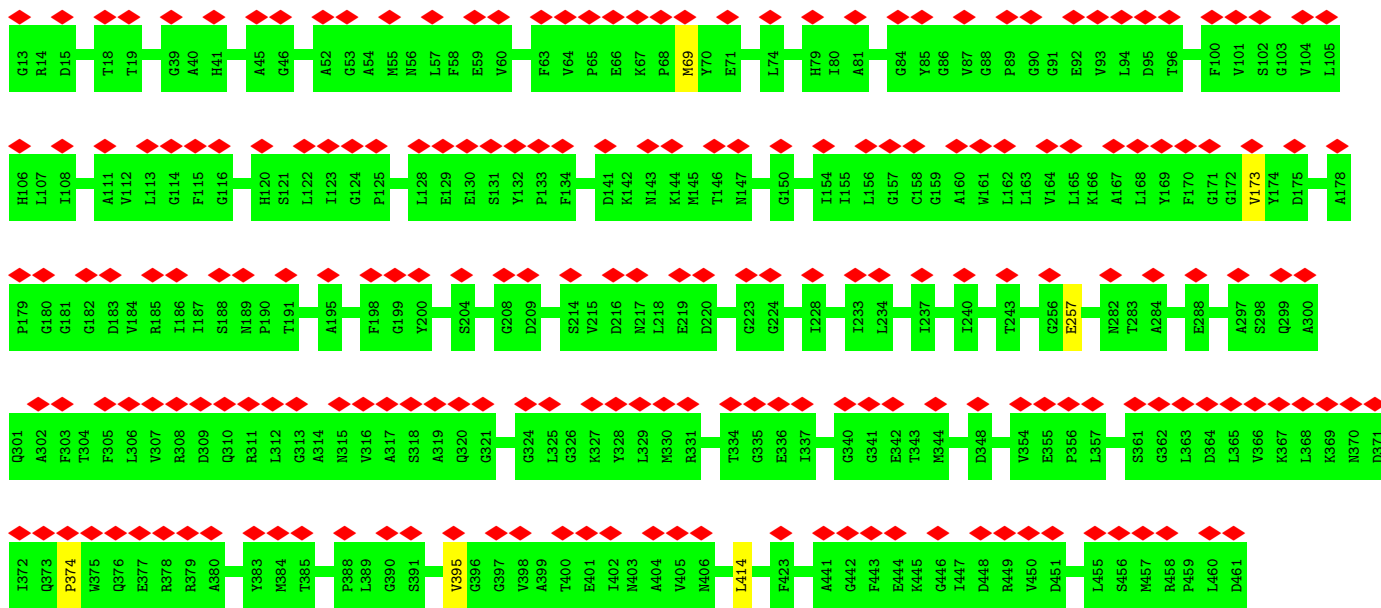


• Molecule 4: Photosystem II CP43 reaction center protein

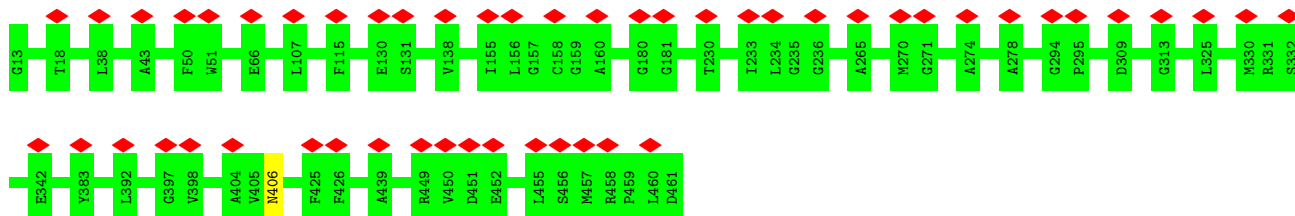




• Molecule 4: Photosystem II CP43 reaction center protein



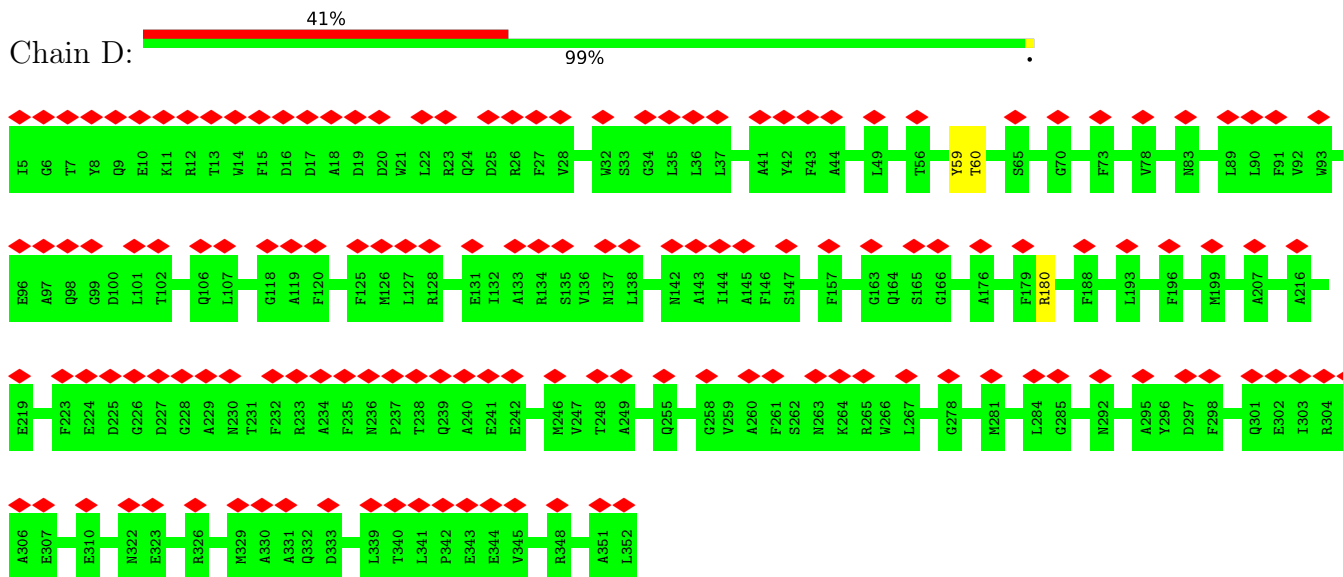
• Molecule 4: Photosystem II CP43 reaction center protein



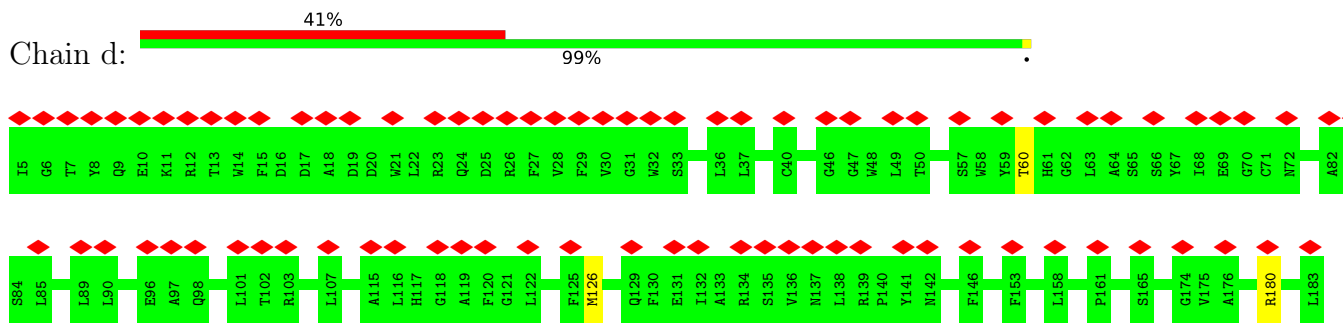
• Molecule 4: Photosystem II CP43 reaction center protein

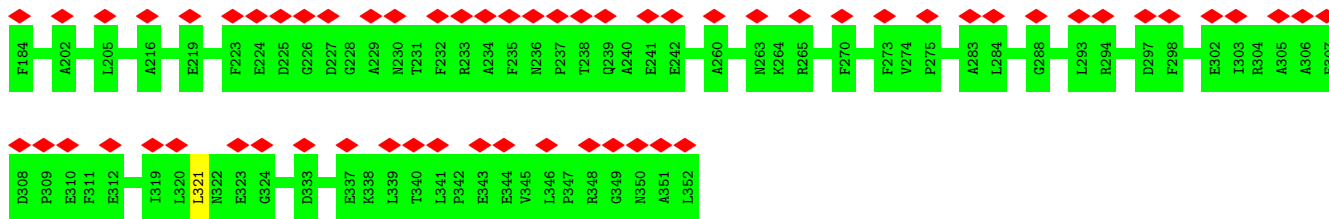


• Molecule 5: Photosystem II D2 protein

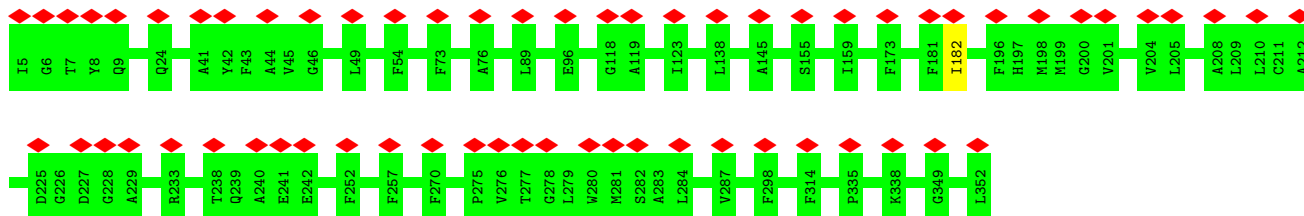


• Molecule 5: Photosystem II D2 protein

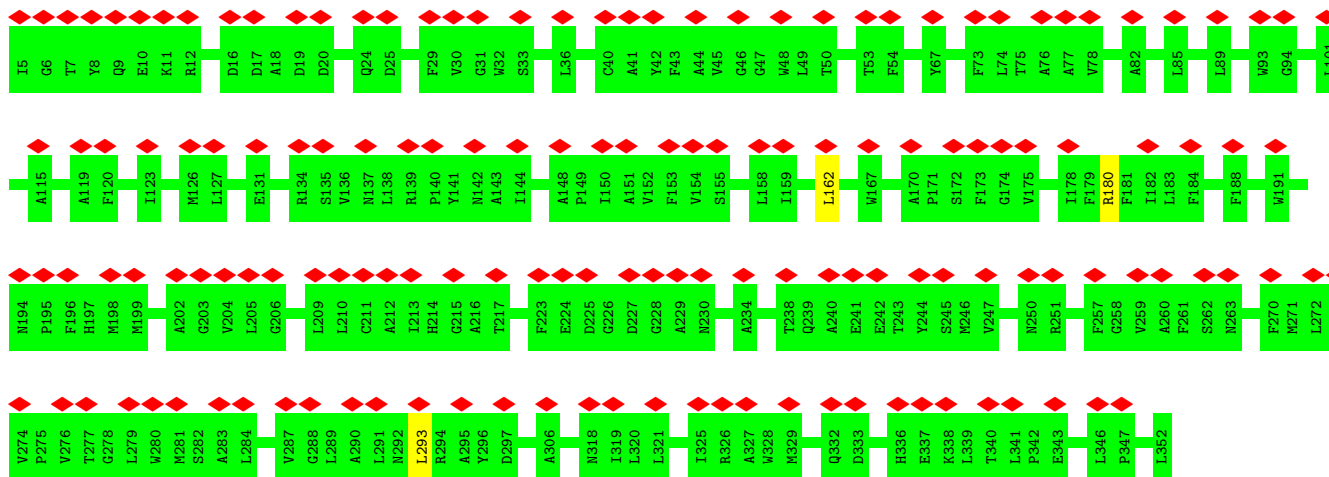
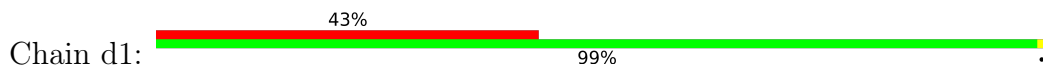




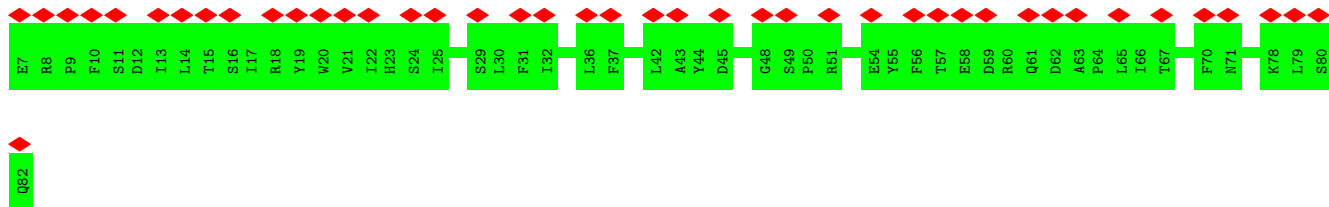
• Molecule 5: Photosystem II D2 protein



• Molecule 5: Photosystem II D2 protein

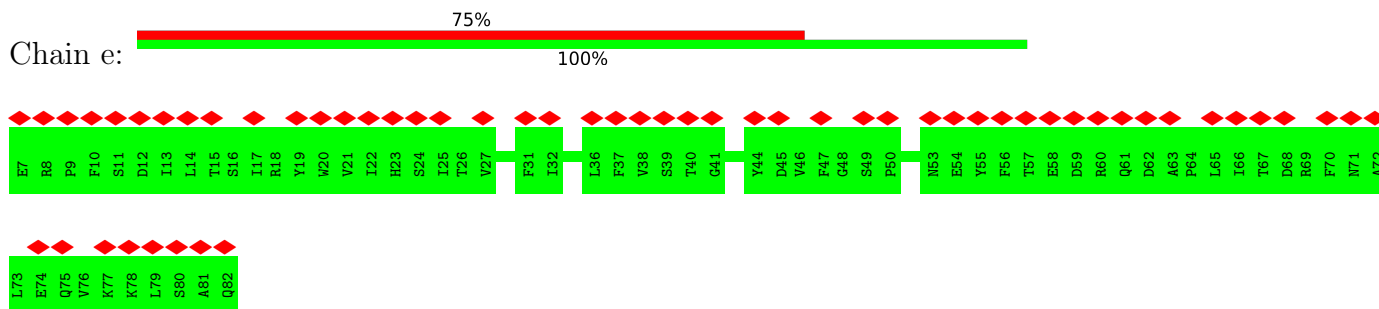


• Molecule 6: Cytochrome b559 subunit alpha

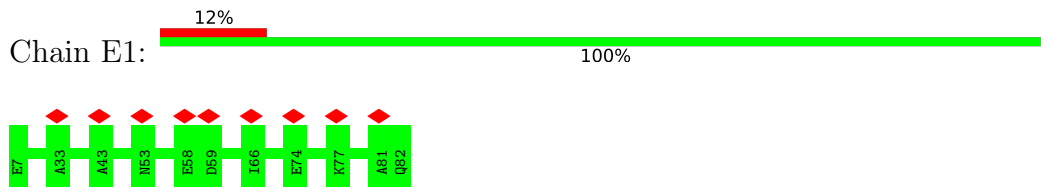


• Molecule 6: Cytochrome b559 subunit alpha

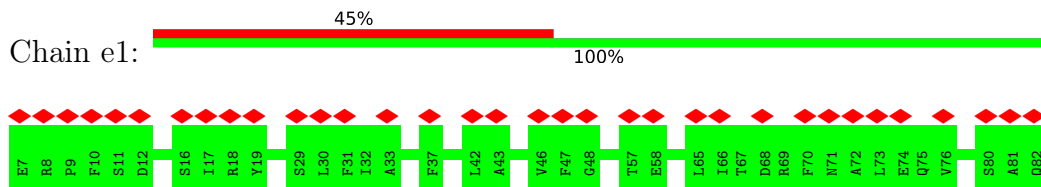




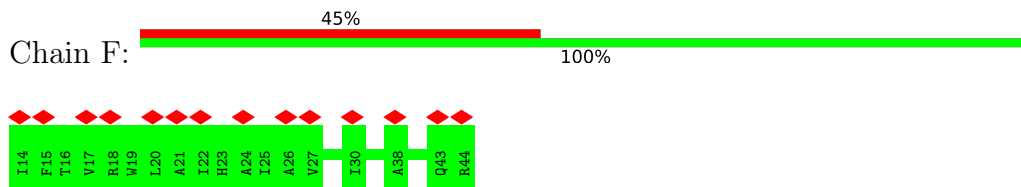
- Molecule 6: Cytochrome b559 subunit alpha



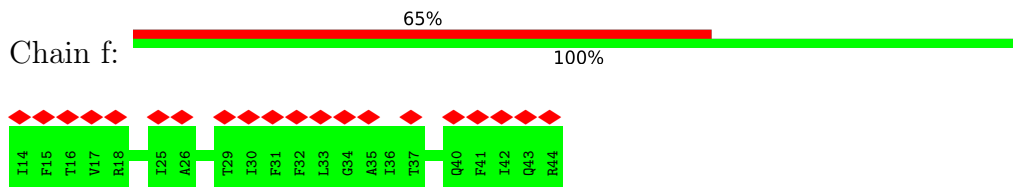
- Molecule 6: Cytochrome b559 subunit alpha



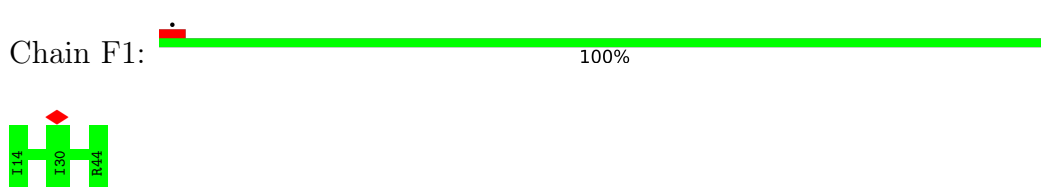
- Molecule 7: Cytochrome b559 subunit beta



- Molecule 7: Cytochrome b559 subunit beta

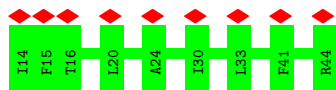


- Molecule 7: Cytochrome b559 subunit beta

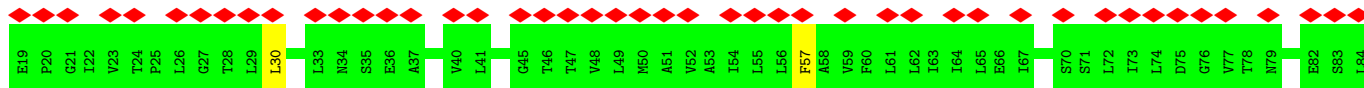


- Molecule 7: Cytochrome b559 subunit beta

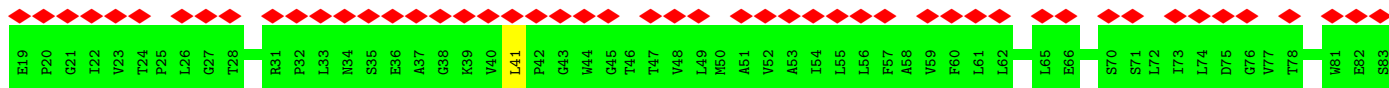
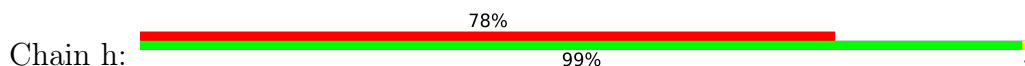




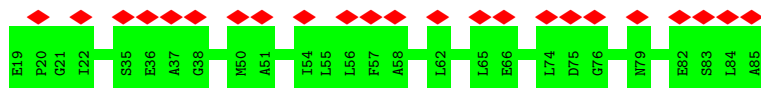
• Molecule 8: Photosystem II reaction center protein H



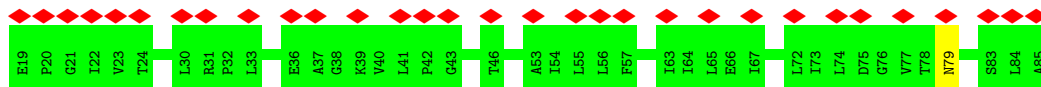
• Molecule 8: Photosystem II reaction center protein H



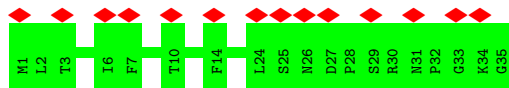
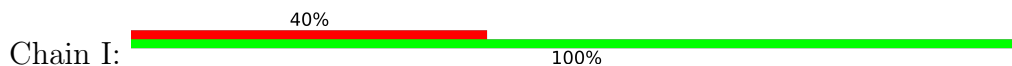
• Molecule 8: Photosystem II reaction center protein H



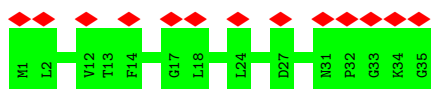
• Molecule 8: Photosystem II reaction center protein H



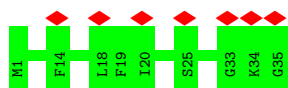
• Molecule 9: Photosystem II reaction center protein I



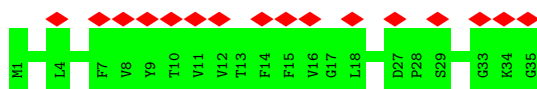
• Molecule 9: Photosystem II reaction center protein I



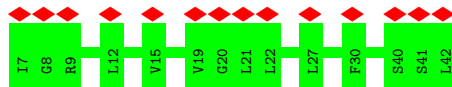
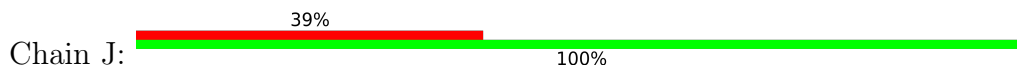
- Molecule 9: Photosystem II reaction center protein I



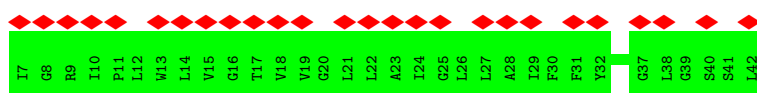
- Molecule 9: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J

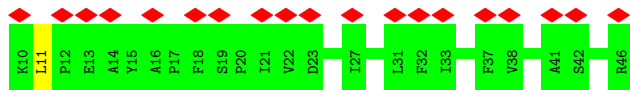


- Molecule 10: Photosystem II reaction center protein J





• Molecule 11: Photosystem II reaction center protein K



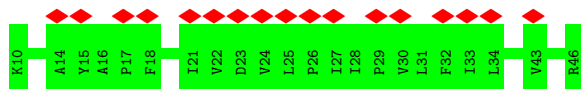
• Molecule 11: Photosystem II reaction center protein K



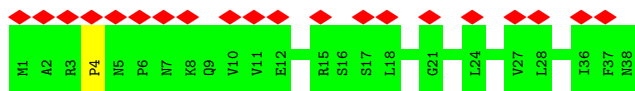
• Molecule 11: Photosystem II reaction center protein K



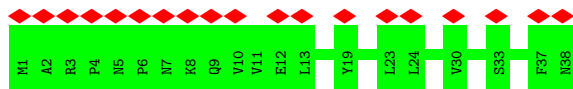
• Molecule 11: Photosystem II reaction center protein K



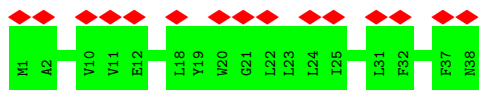
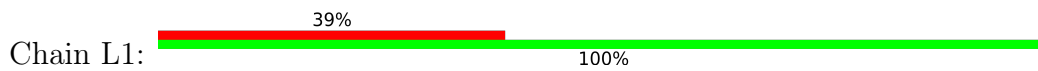
• Molecule 12: Photosystem II reaction center protein L



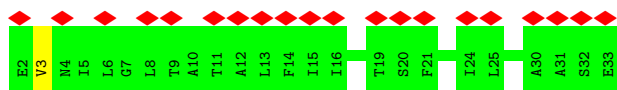
• Molecule 12: Photosystem II reaction center protein L



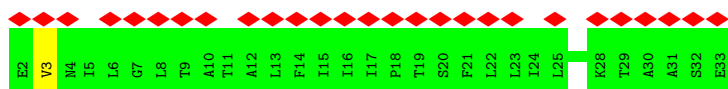
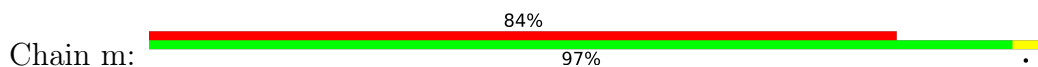
• Molecule 12: Photosystem II reaction center protein L



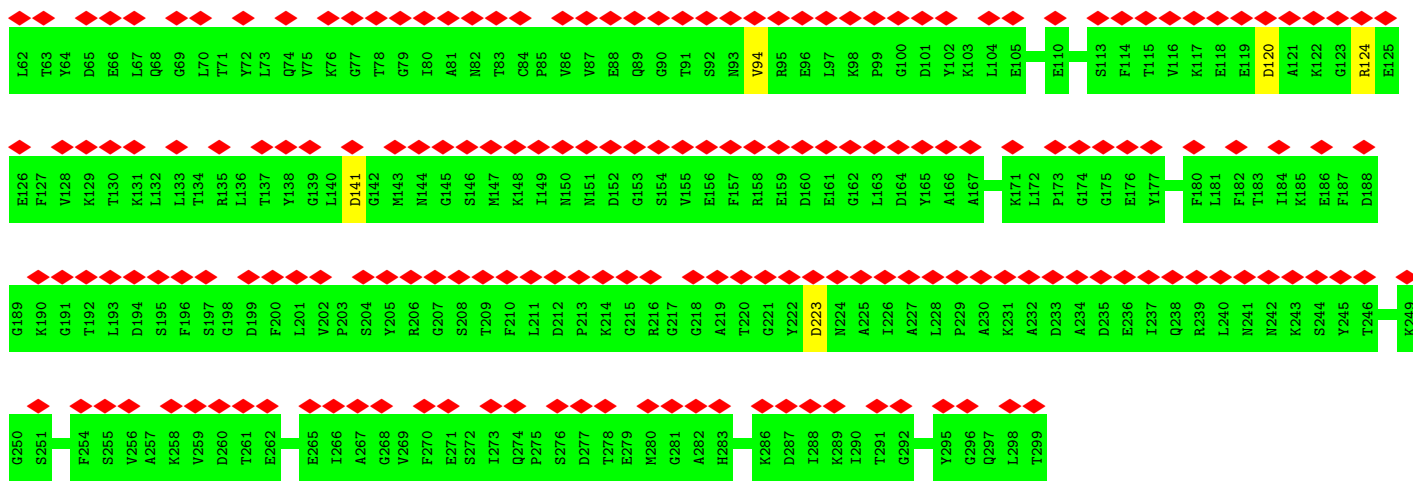
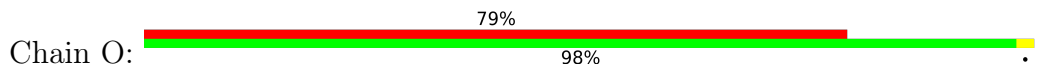
• Molecule 13: Photosystem II reaction center protein M



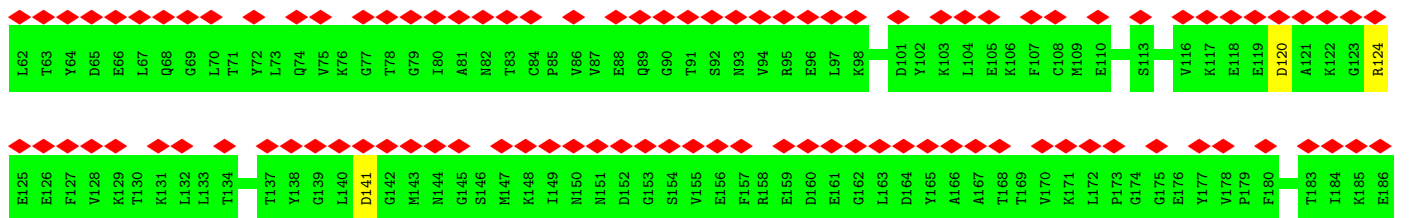
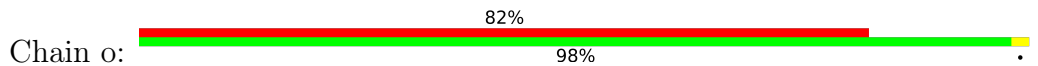
• Molecule 13: Photosystem II reaction center protein M

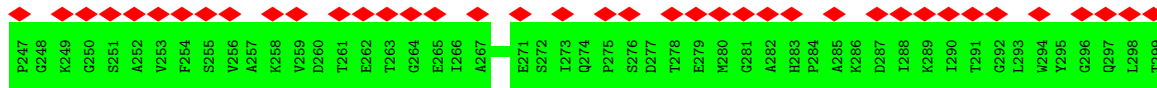
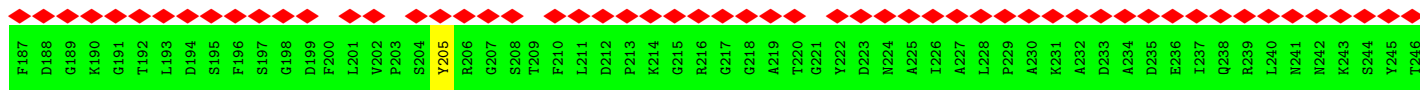


• Molecule 14: PsbO

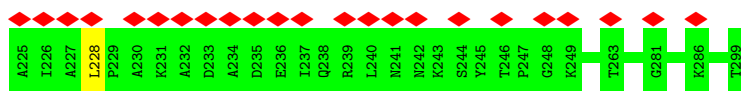
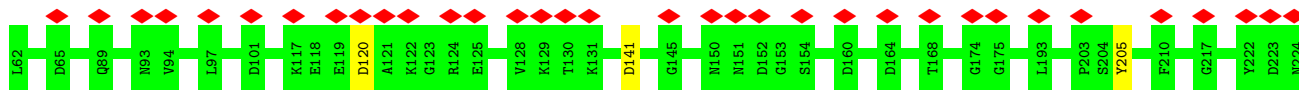


• Molecule 14: PsbO

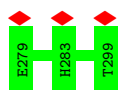
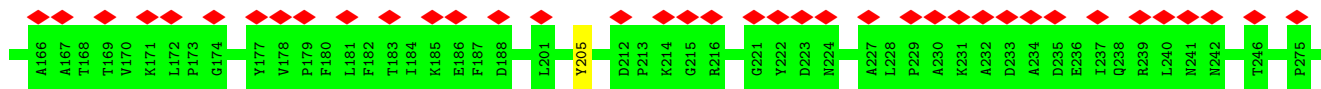




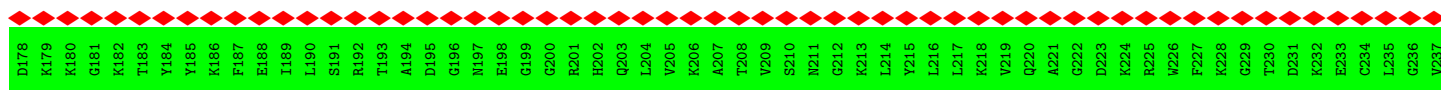
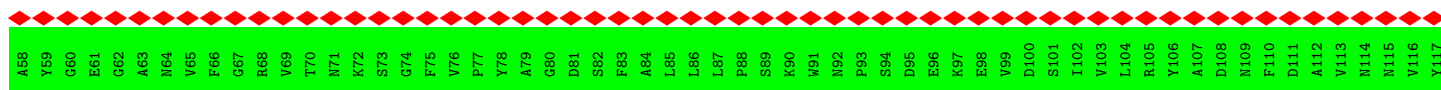
• Molecule 14: PsbO



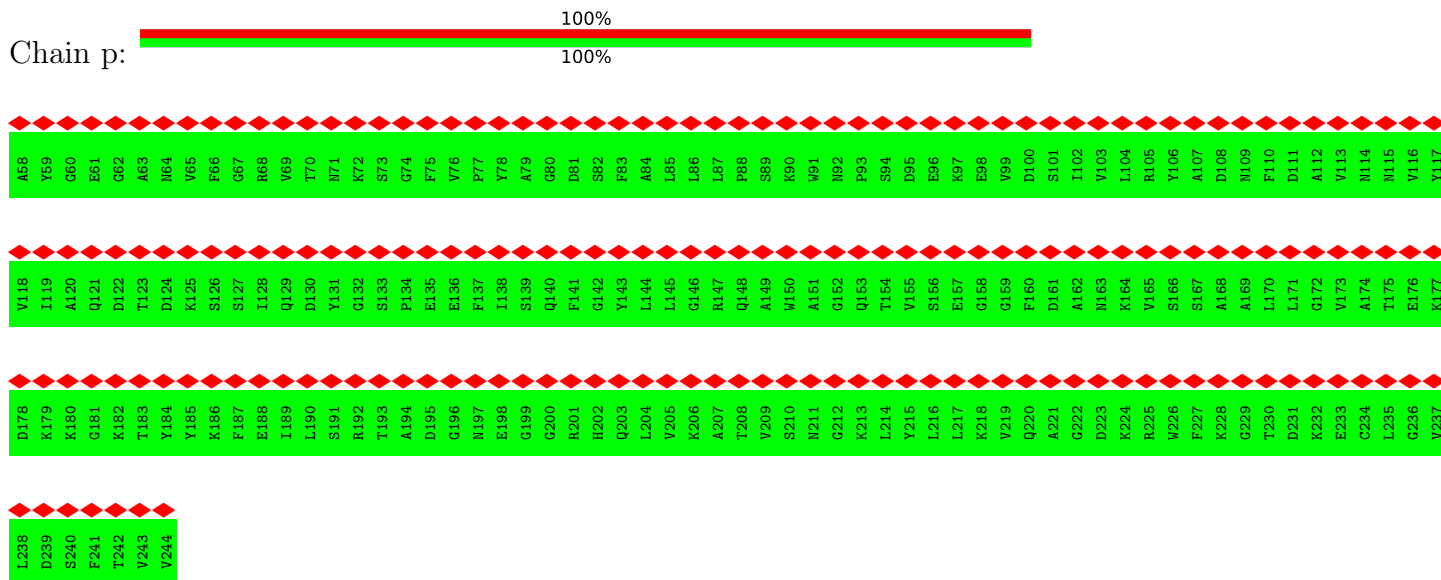
• Molecule 14: PsbO



• Molecule 15: PsbP



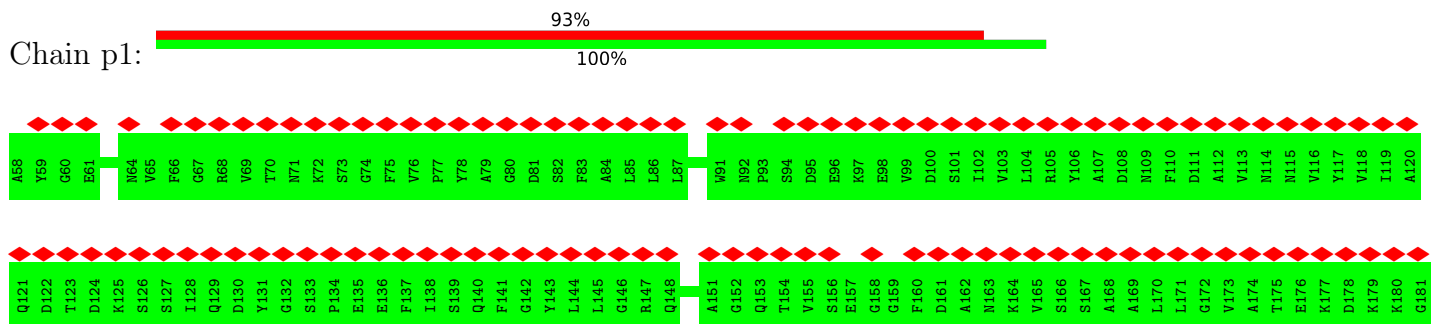
• Molecule 15: PspB

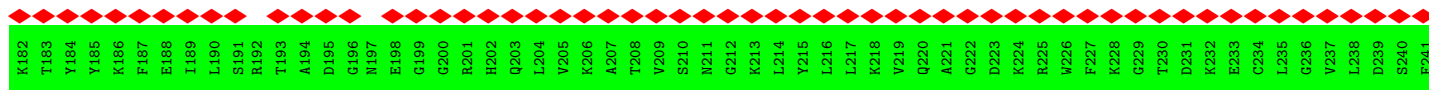


• Molecule 15: PspB

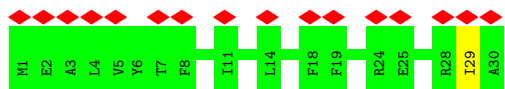


• Molecule 15: PspB

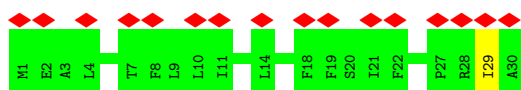




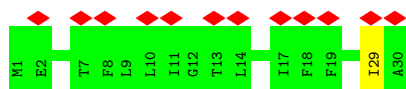
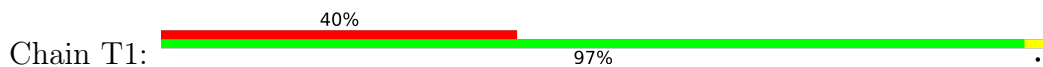
• Molecule 16: Photosystem II reaction center protein T



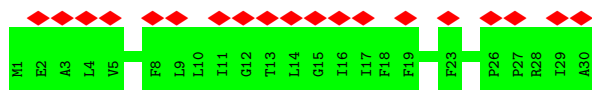
• Molecule 16: Photosystem II reaction center protein T



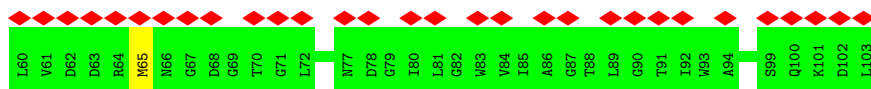
• Molecule 16: Photosystem II reaction center protein T



• Molecule 16: Photosystem II reaction center protein T



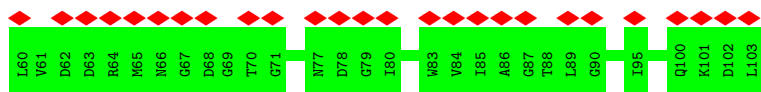
• Molecule 17: PsbW



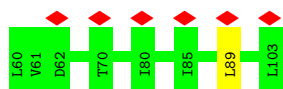
• Molecule 17: PsbW



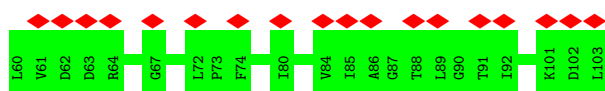
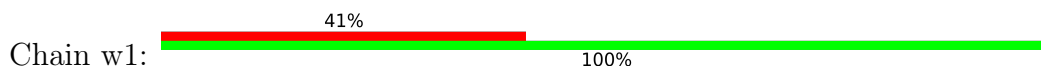




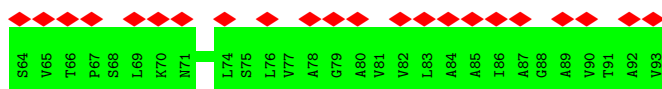
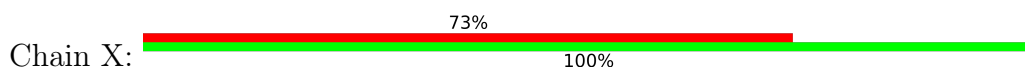
• Molecule 17: PsbW



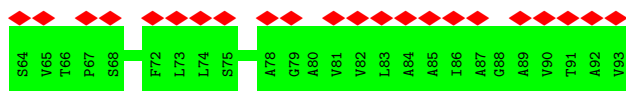
• Molecule 17: PsbW



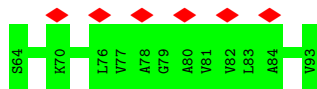
• Molecule 18: PsbX



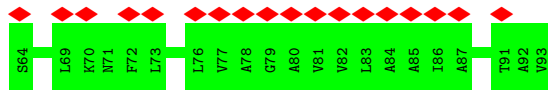
• Molecule 18: PsbX



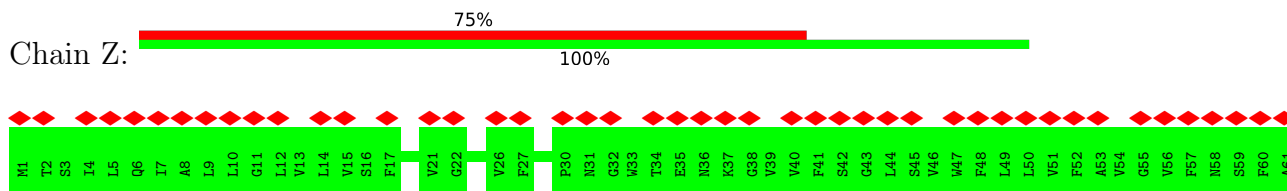
• Molecule 18: PsbX



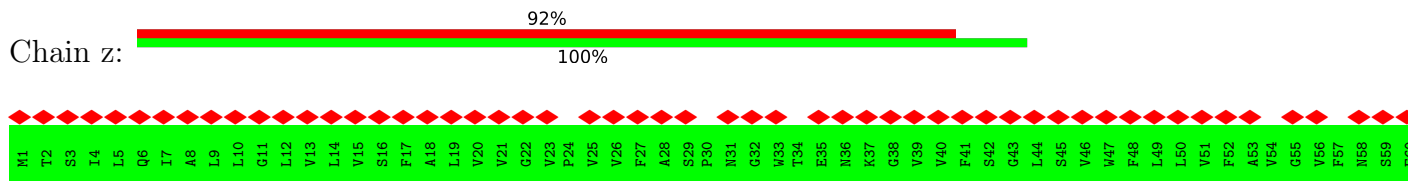
• Molecule 18: PsbX



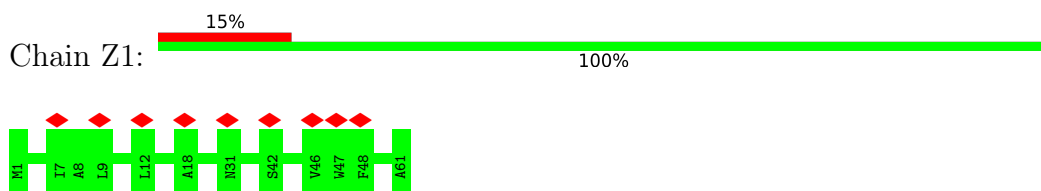
• Molecule 19: PsbZ



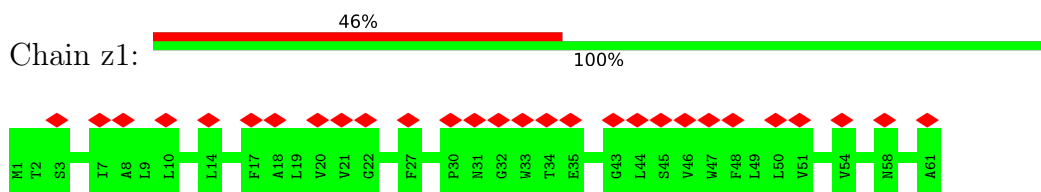
• Molecule 19: PsbZ



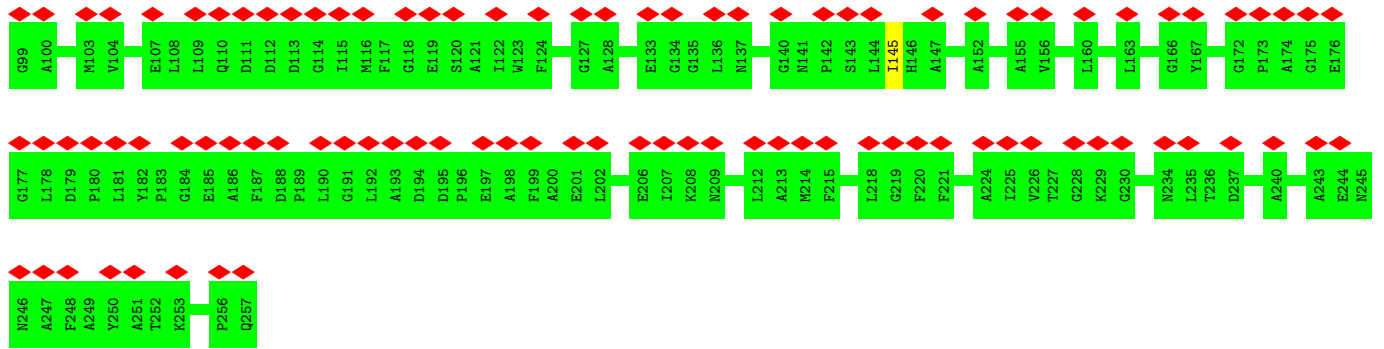
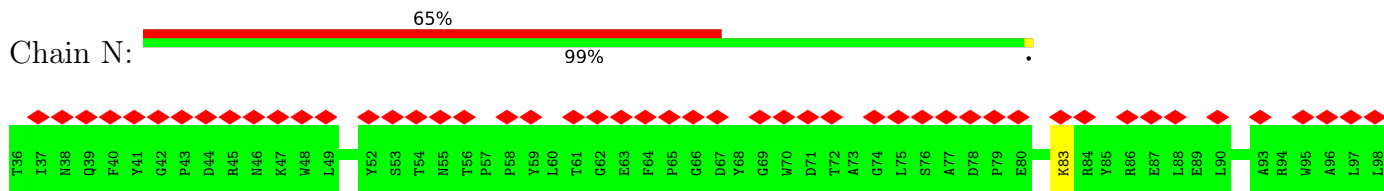
• Molecule 19: PsbZ



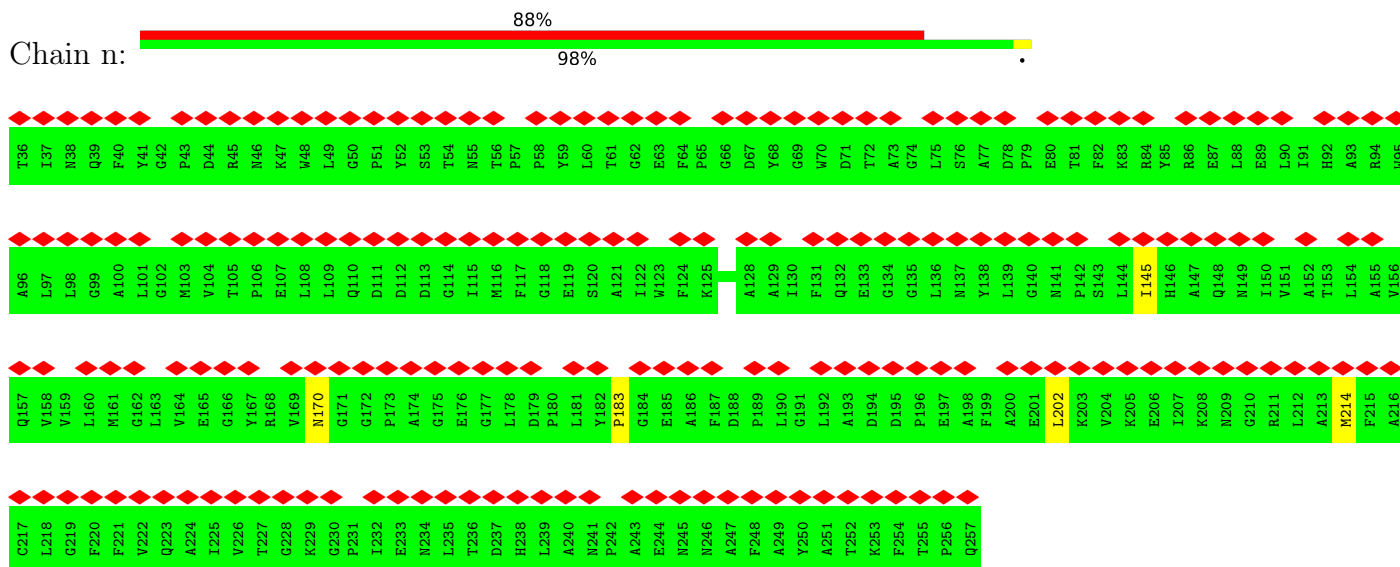
• Molecule 19: PsbZ



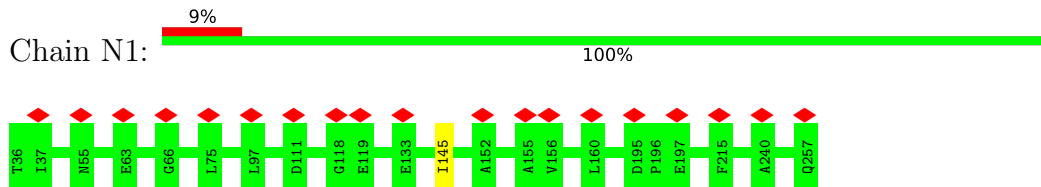
• Molecule 20: LHCII M3



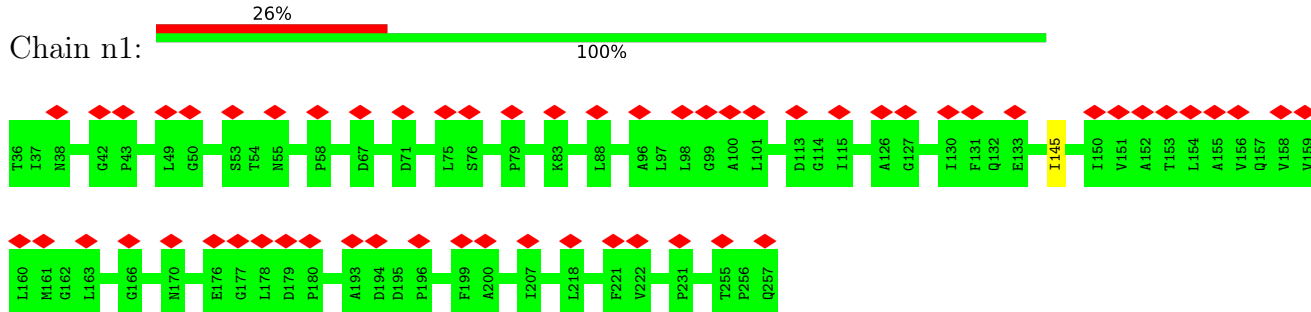
• Molecule 20: LHCII M3



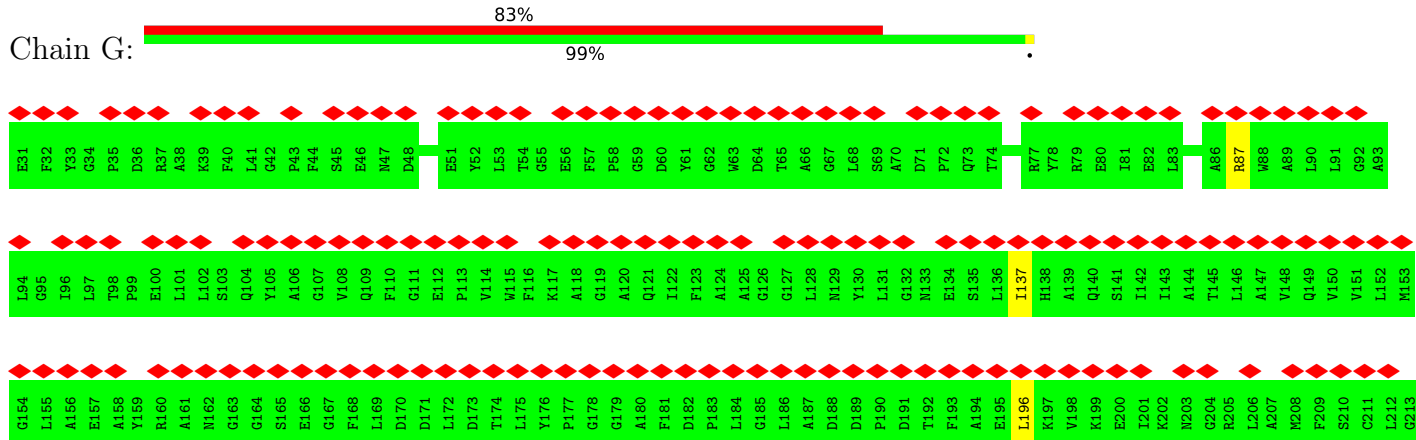
• Molecule 20: LHCII M3

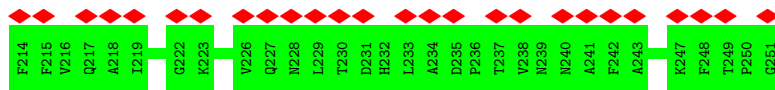


• Molecule 20: LHCII M3

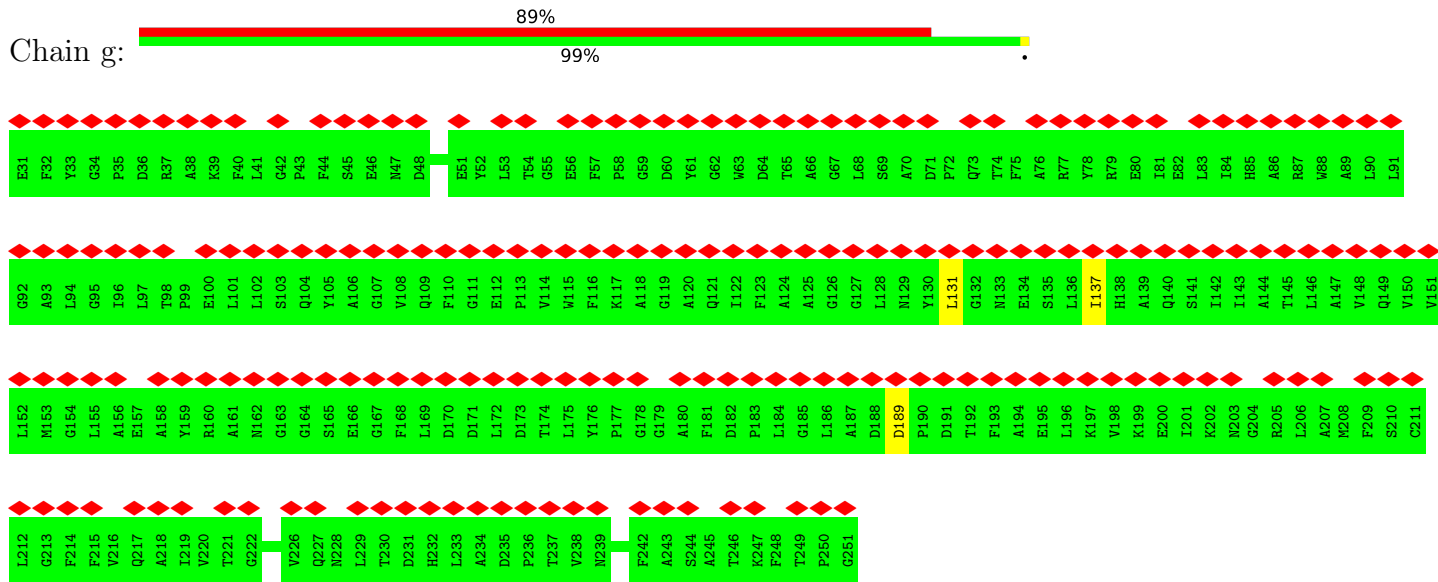


• Molecule 21: LHCII M2

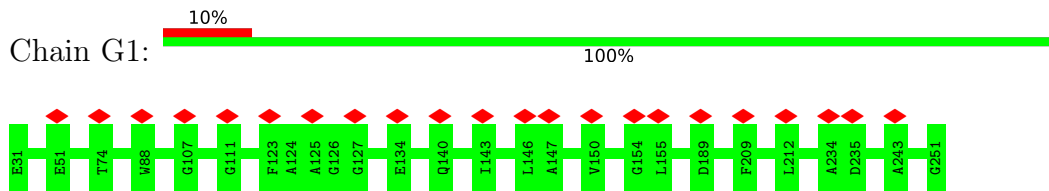




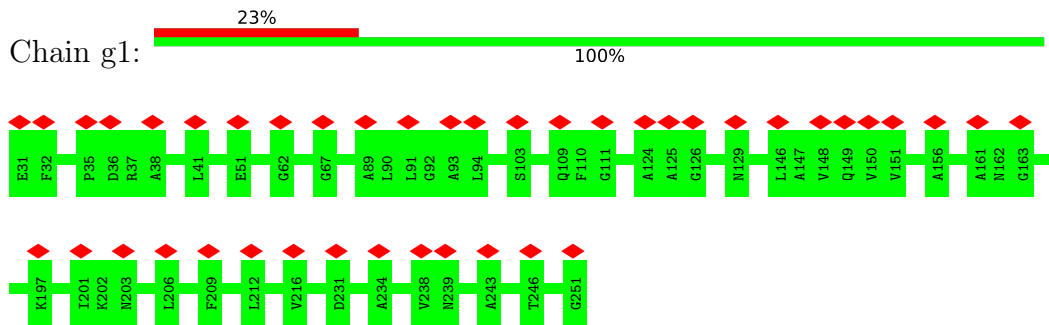
• Molecule 21: LHCII M2



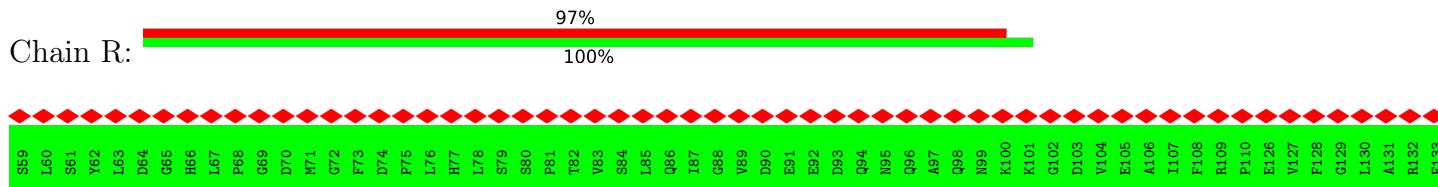
• Molecule 21: LHCII M2

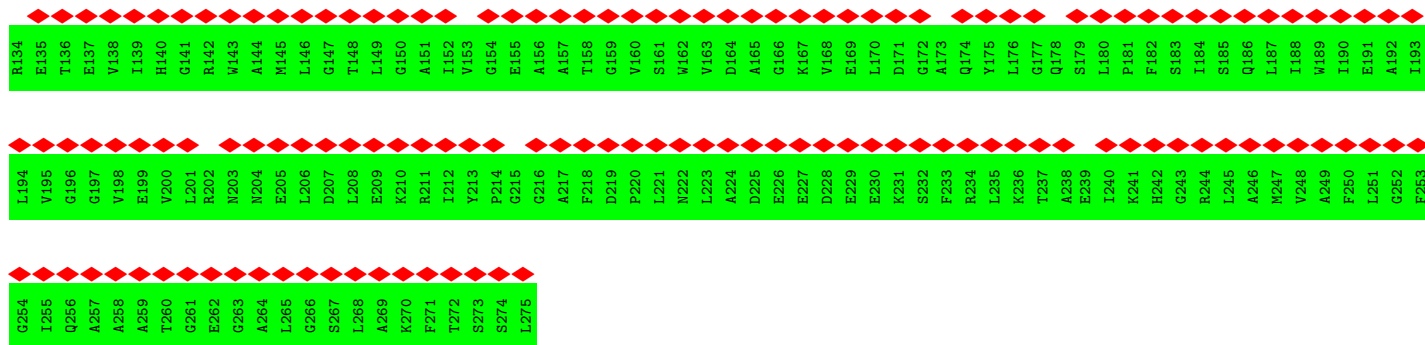


• Molecule 21: LHCII M2

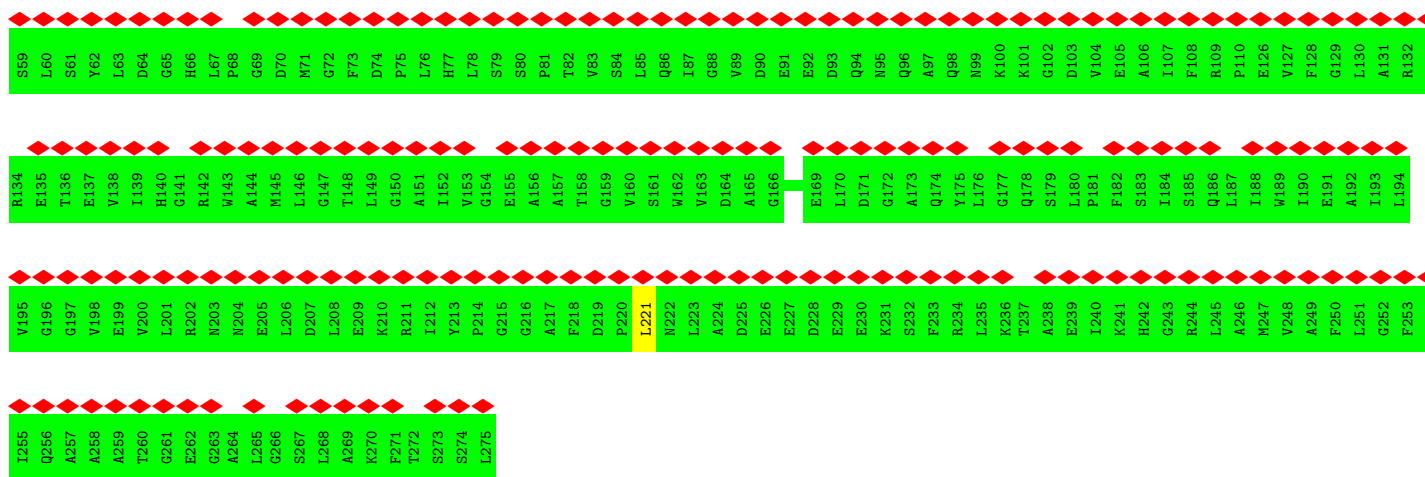
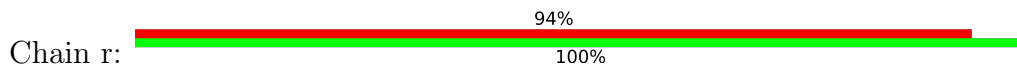


• Molecule 22: CP29

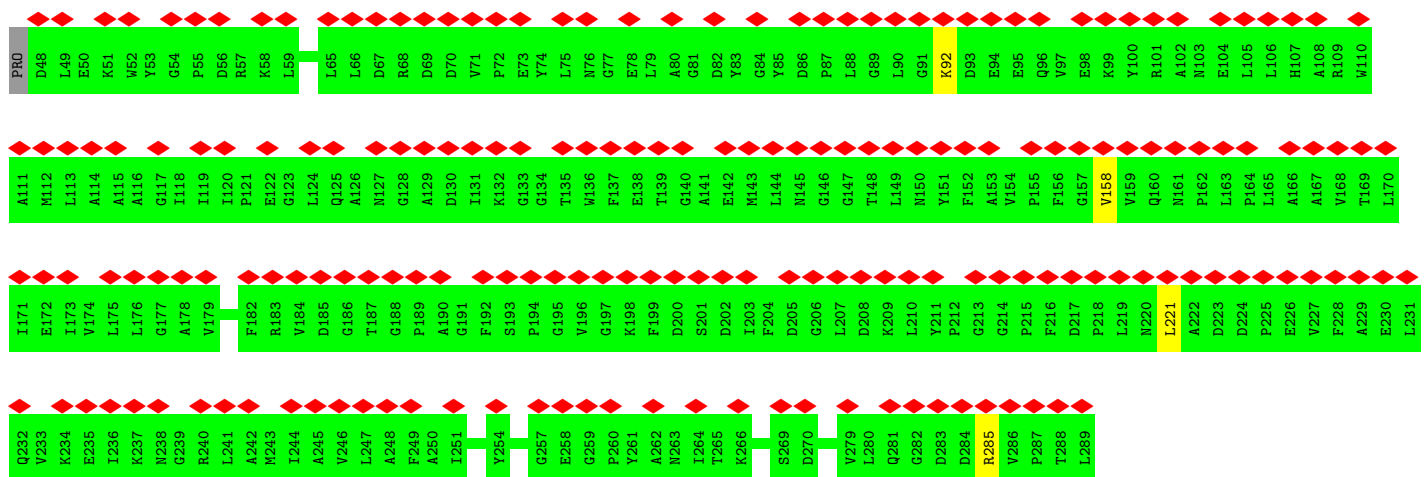
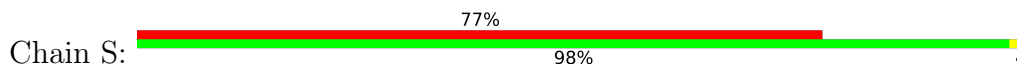




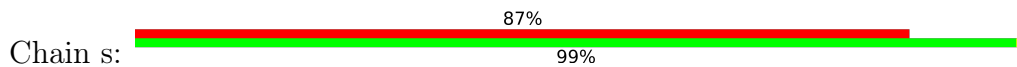
• Molecule 22: CP29

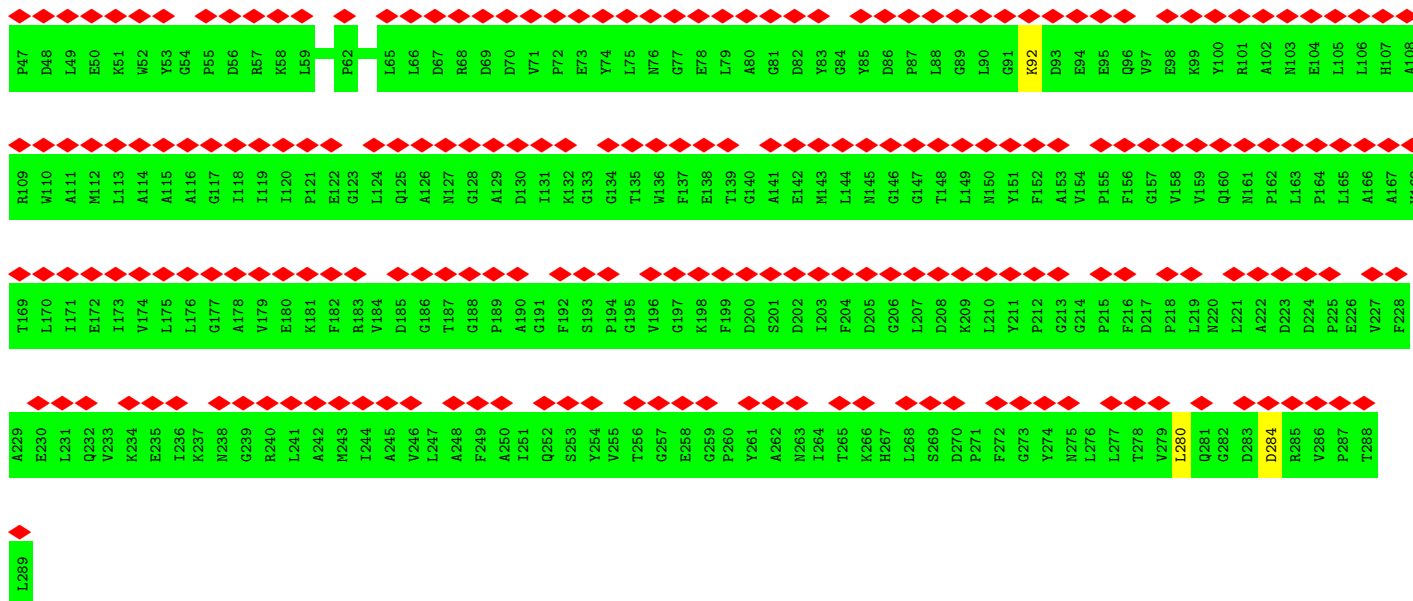


• Molecule 23: CP26

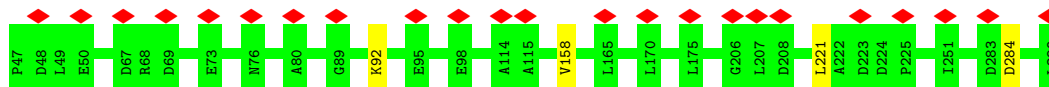


• Molecule 23: CP26

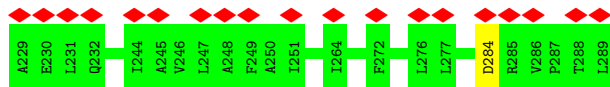
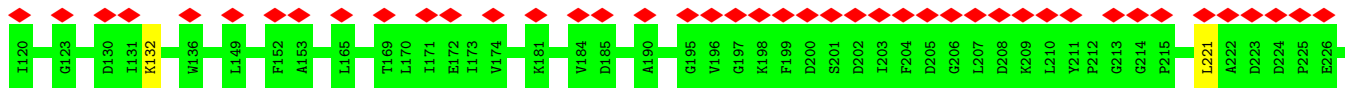
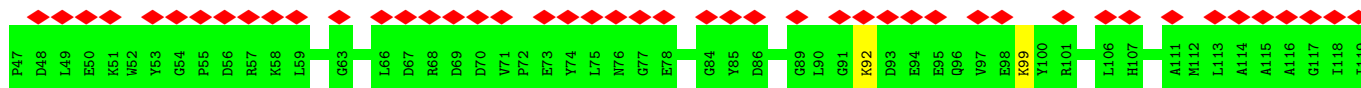
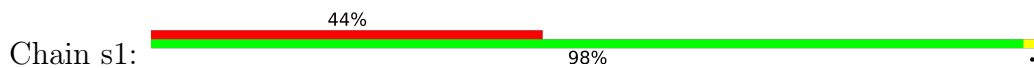




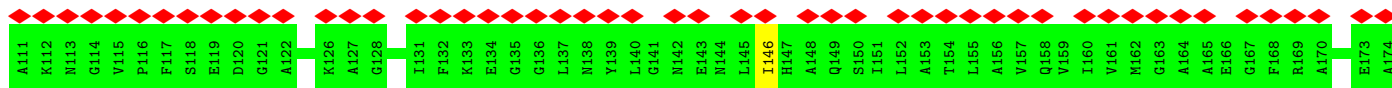
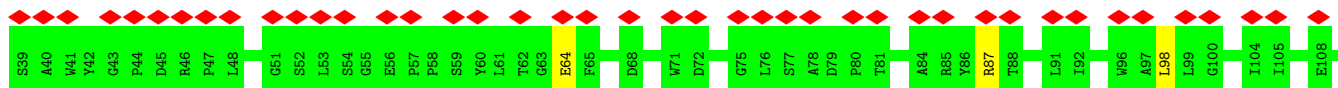
• Molecule 23: CP26

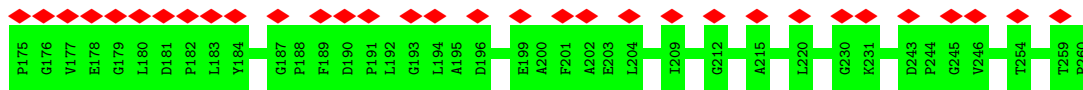


• Molecule 23: CP26

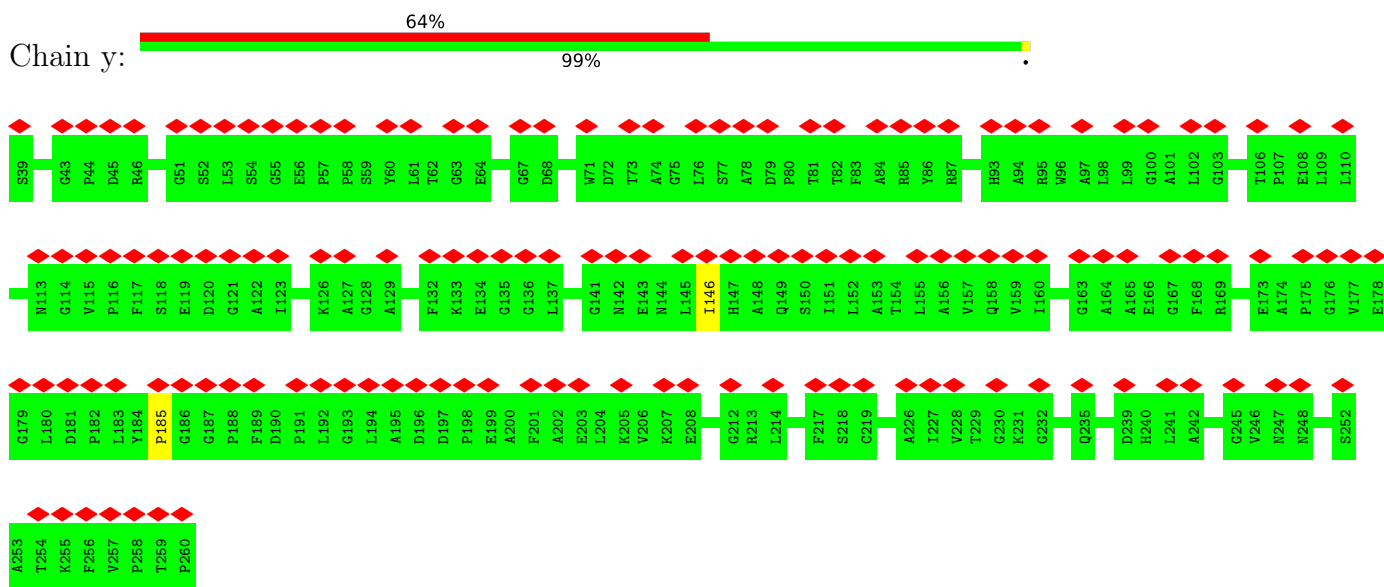


• Molecule 24: LHCII M1

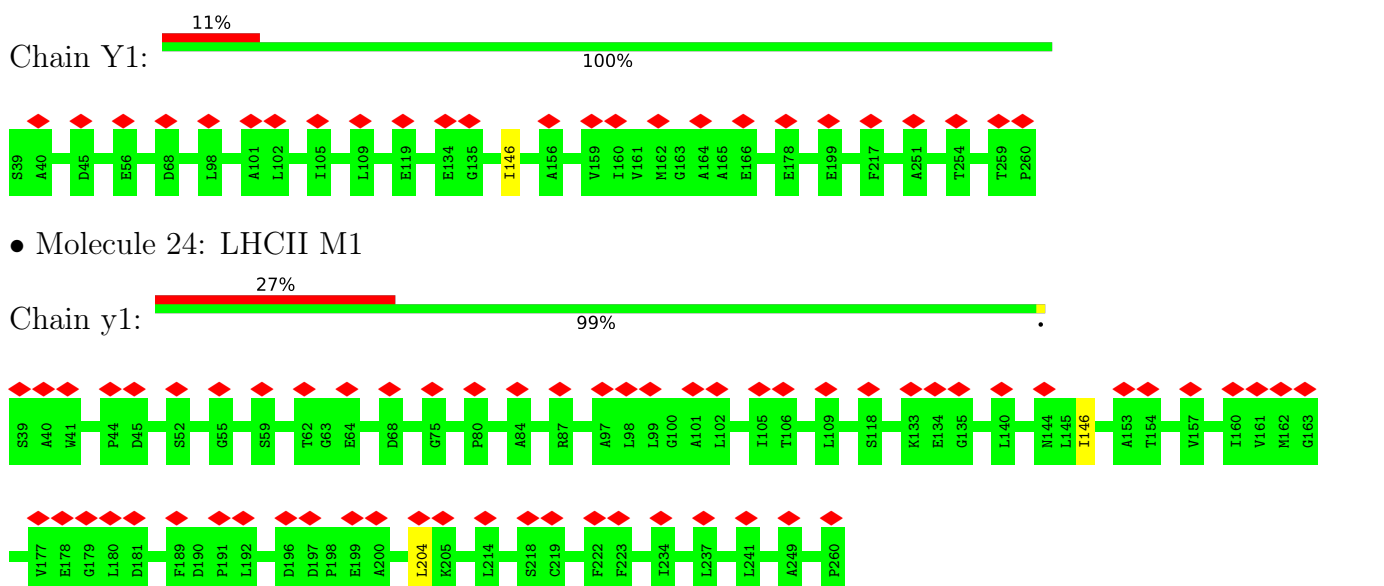




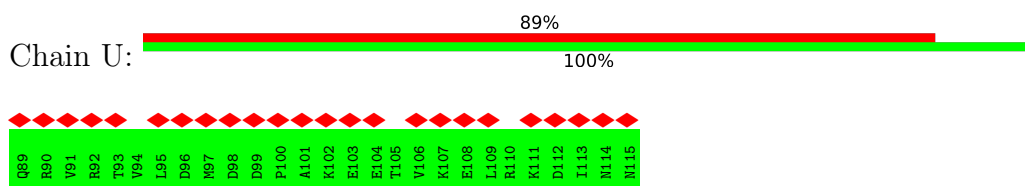
• Molecule 24: LHCII M1



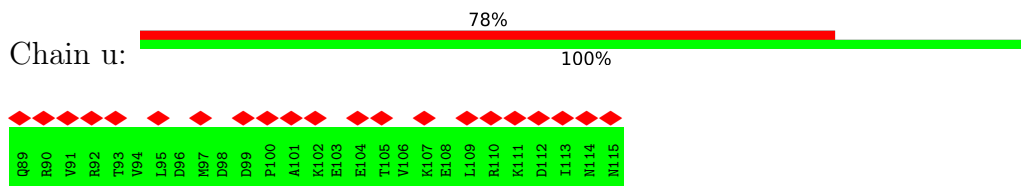
• Molecule 24: LHCII M1



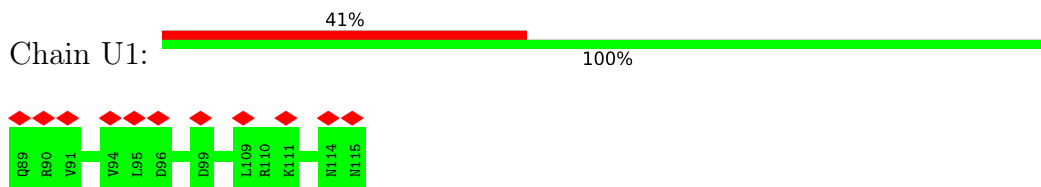
• Molecule 25: PsbU



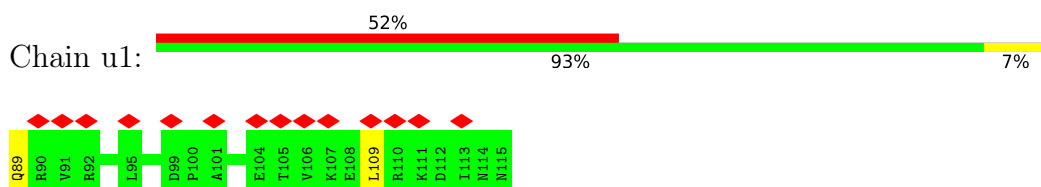
• Molecule 25: PsbU



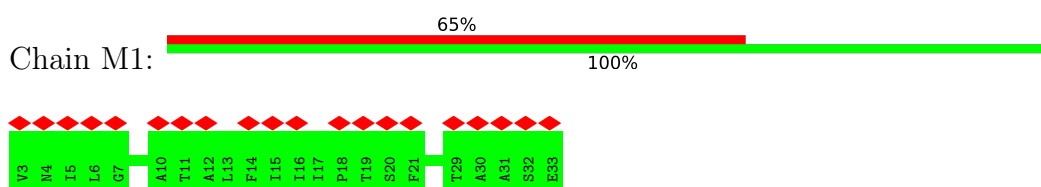
• Molecule 25: PsbU



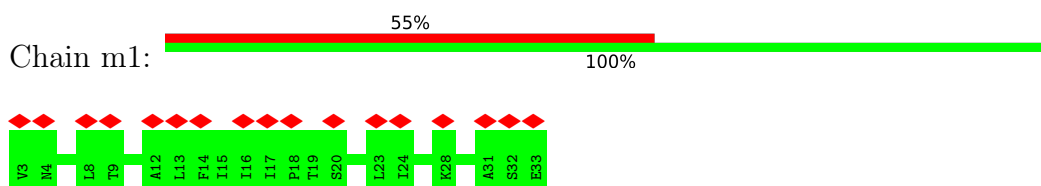
• Molecule 25: PsbU



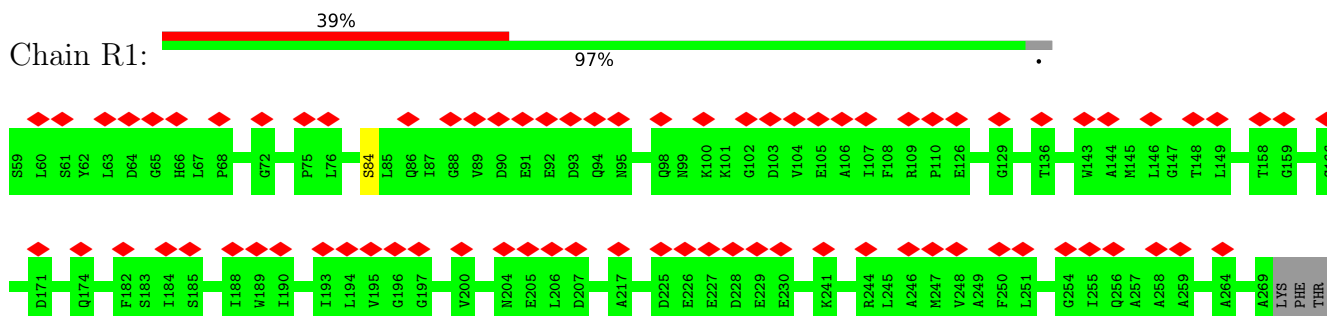
• Molecule 26: Photosystem II reaction center protein M



• Molecule 26: Photosystem II reaction center protein M



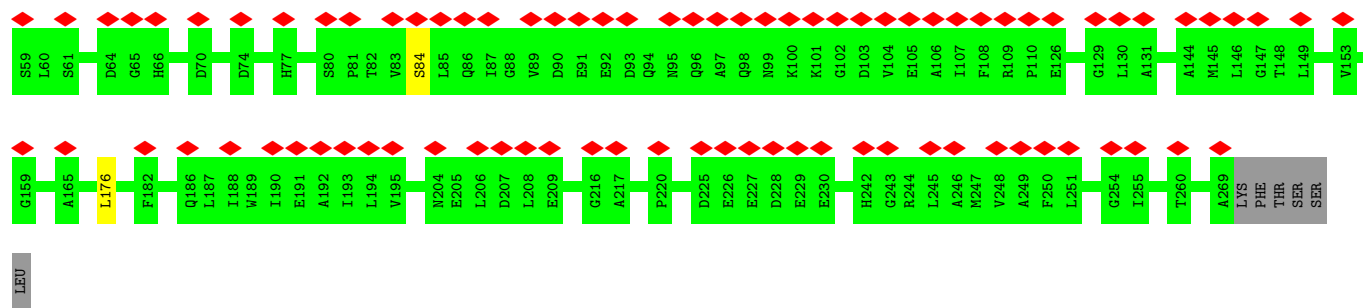
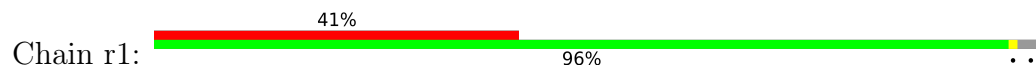
• Molecule 27: CP29



SER SER LEU

• Molecule 27: CP29





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0175	Depositor
Map size ( $\text{\AA}$ )	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.96, 0.96, 0.96	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, LPX, PTY, DGD, CHL, LMG, DGA, NEX, RRX, HEM, GOL, LMK, LUT, PL9, 4RF, SEP, CL, CLA, FE2, 3PH, SQD, SPH, NA, PHO, C7Z, XAT, ERG, LHG, BCT, OEX, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/2723	0.61	1/3715 (0.0%)
1	A1	0.31	0/2723	0.59	1/3715 (0.0%)
1	a	0.35	0/2723	0.63	1/3715 (0.0%)
1	a1	0.31	1/2723 (0.0%)	0.59	3/3715 (0.1%)
2	B	0.40	2/3912 (0.1%)	0.66	6/5327 (0.1%)
2	B1	0.29	0/3912	0.56	2/5327 (0.0%)
2	b	0.31	0/3912	0.59	0/5327
2	b1	0.29	0/3912	0.56	0/5327
3	V	0.26	0/228	0.58	0/311
3	V1	0.25	0/228	0.65	0/311
3	v	0.28	0/228	0.57	0/311
3	v1	0.24	0/228	0.58	0/311
4	C	0.32	0/3602	0.59	1/4913 (0.0%)
4	C1	0.29	0/3602	0.55	0/4913
4	c	0.43	1/3602 (0.0%)	0.74	6/4913 (0.1%)
4	c1	0.32	0/3602	0.57	1/4913 (0.0%)
5	D	0.32	0/2860	0.62	1/3899 (0.0%)
5	D1	0.30	0/2860	0.59	1/3899 (0.0%)
5	d	0.33	0/2860	0.62	3/3899 (0.1%)
5	d1	0.30	0/2860	0.58	2/3899 (0.1%)
6	E	0.30	0/639	0.57	0/870
6	E1	0.27	0/639	0.53	0/870
6	e	0.30	0/639	0.59	0/870
6	e1	0.26	0/639	0.51	0/870
7	F	0.28	0/259	0.59	0/351
7	F1	0.29	0/259	0.53	0/351
7	f	0.27	0/259	0.54	0/351
7	f1	0.25	0/259	0.49	0/351
8	H	6.04	6/513 (1.2%)	0.91	5/703 (0.7%)
8	H1	0.26	0/513	0.60	0/703
8	h	0.31	0/513	0.66	1/703 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	h1	0.28	0/513	0.56	0/703
9	I	0.31	0/287	0.60	0/386
9	I1	0.35	0/287	0.66	0/386
9	i	0.32	0/287	0.65	0/386
9	i1	0.27	0/287	0.50	0/386
10	J	0.26	0/272	0.54	0/369
10	J1	0.26	0/272	0.55	0/369
10	j	0.26	0/272	0.50	0/369
10	j1	0.27	0/272	0.56	0/369
11	K	0.36	0/308	0.69	1/423 (0.2%)
11	K1	0.32	0/308	0.65	1/423 (0.2%)
11	k	0.36	0/308	0.66	0/423
11	k1	0.37	0/308	0.63	0/423
12	L	0.43	0/321	0.73	1/435 (0.2%)
12	L1	0.29	0/321	0.64	0/435
12	l	0.31	0/321	0.55	0/435
13	M	0.29	0/246	0.55	0/335
13	m	0.29	0/246	0.66	0/335
14	O	0.30	0/1855	0.64	3/2505 (0.1%)
14	O1	0.28	0/1855	0.64	3/2505 (0.1%)
14	o	0.29	0/1855	0.61	2/2505 (0.1%)
14	o1	0.29	0/1855	0.66	3/2505 (0.1%)
15	P	0.28	0/1473	0.56	0/1988
15	P1	0.27	0/1473	0.57	0/1988
15	p	0.26	0/1473	0.51	0/1988
15	p1	0.26	0/1473	0.54	0/1988
16	T	0.30	0/254	0.57	0/342
16	T1	0.29	0/254	0.56	0/342
16	t	0.32	0/254	0.62	0/342
16	t1	0.29	0/254	0.65	0/342
17	W	0.29	0/339	0.54	0/460
17	W1	0.26	0/339	0.60	1/460 (0.2%)
17	w	0.28	0/339	0.52	0/460
17	w1	0.25	0/339	0.52	0/460
18	X	0.25	0/202	0.53	0/276
18	X1	0.28	0/202	0.49	0/276
18	x	0.28	0/202	0.58	0/276
18	x1	0.28	0/202	0.42	0/276
19	Z	0.29	0/469	0.58	0/641
19	Z1	0.26	0/469	0.48	0/641
19	z	0.27	0/469	0.46	0/641
19	z1	0.28	0/469	0.48	0/641
20	N	0.31	0/1751	0.60	0/2386

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	N1	0.30	0/1751	0.55	0/2386
20	n	0.33	0/1751	0.67	2/2386 (0.1%)
20	n1	0.27	0/1750	0.52	0/2382
21	G	0.31	0/1725	0.62	1/2348 (0.0%)
21	G1	0.28	0/1725	0.54	0/2348
21	g	0.31	0/1725	0.59	2/2348 (0.1%)
21	g1	0.28	0/1725	0.54	0/2348
22	R	0.27	0/1561	0.57	0/2110
22	r	0.28	0/1561	0.59	1/2110 (0.0%)
23	S	0.30	0/1895	0.59	1/2579 (0.0%)
23	S1	0.27	0/1903	0.56	1/2590 (0.0%)
23	s	0.28	0/1902	0.57	1/2587 (0.0%)
23	s1	0.27	0/1903	0.54	1/2590 (0.0%)
24	Y	0.38	0/1715	0.71	3/2338 (0.1%)
24	Y1	0.32	0/1715	0.56	0/2338
24	y	0.45	2/1715 (0.1%)	0.75	4/2338 (0.2%)
24	y1	0.28	0/1715	0.54	1/2338 (0.0%)
25	U	0.25	0/224	0.66	0/298
25	U1	0.30	0/224	0.61	0/298
25	u	0.32	0/224	0.79	0/298
25	u1	0.30	0/224	0.70	1/298 (0.3%)
26	M1	0.27	0/237	0.57	0/323
26	m1	0.27	0/237	0.48	0/323
27	R1	0.26	0/1506	0.52	0/2035
27	r1	0.27	0/1506	0.59	1/2035 (0.0%)
All	All	0.50	12/118105 (0.0%)	0.60	70/160649 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	57	PHE	CE2-CZ	63.39	2.57	1.37
8	H	57	PHE	CD2-CE2	62.87	2.65	1.39
8	H	57	PHE	CE1-CZ	62.87	2.56	1.37
8	H	57	PHE	CD1-CE1	61.06	2.61	1.39
8	H	57	PHE	CG-CD2	38.86	1.97	1.38
8	H	57	PHE	CG-CD1	38.74	1.96	1.38
4	c	374	PRO	CG-CD	-14.57	1.02	1.50
2	B	88	PRO	CG-CD	-11.75	1.11	1.50
24	y	185	PRO	CG-CD	-11.04	1.14	1.50
2	B	50	PRO	CG-CD	-7.32	1.26	1.50
24	y	185	PRO	CB-CG	-7.12	1.14	1.50
1	a1	39	PRO	CG-CD	-5.05	1.33	1.50

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	185	PRO	N-CD-CG	-17.70	76.65	103.20
4	c	374	PRO	N-CD-CG	-16.63	78.26	103.20
2	B	88	PRO	N-CD-CG	-13.67	82.69	103.20
24	y	185	PRO	CA-CB-CG	-11.49	82.17	104.00
2	B	50	PRO	CA-N-CD	-10.86	96.29	111.50
24	y	185	PRO	CB-CG-CD	10.36	146.92	106.50
2	B	88	PRO	CA-N-CD	-10.16	97.28	111.50
8	H	57	PHE	CB-CG-CD1	-9.30	114.29	120.80
4	c	374	PRO	CA-CB-CG	-9.24	86.45	104.00
2	B	50	PRO	N-CD-CG	-9.07	89.59	103.20
20	n	214	MET	CB-CG-SD	9.04	139.52	112.40
24	Y	87	ARG	CG-CD-NE	-8.95	93.00	111.80
24	Y	64	GLU	C-N-CA	8.92	144.01	121.70
8	H	57	PHE	CD1-CG-CD2	8.66	129.56	118.30
20	n	202	LEU	CA-CB-CG	8.45	134.73	115.30
4	c	374	PRO	CA-N-CD	-8.37	99.78	111.50
1	a1	39	PRO	N-CD-CG	-8.06	91.11	103.20
2	B1	296	LEU	CA-CB-CG	7.79	133.21	115.30
12	L	4	PRO	N-CD-CG	-7.78	91.53	103.20
2	B	88	PRO	CA-CB-CG	-7.40	89.93	104.00
21	G	196	LEU	CA-CB-CG	7.40	132.33	115.30
1	a1	39	PRO	CA-N-CD	-7.24	101.36	111.50
24	y	185	PRO	CA-N-CD	-7.09	101.57	111.50
23	S1	221	LEU	CA-CB-CG	7.00	131.39	115.30
5	d1	293	LEU	CA-CB-CG	6.70	130.72	115.30
8	H	57	PHE	CB-CG-CD2	-6.69	116.12	120.80
23	s1	221	LEU	CA-CB-CG	6.66	130.61	115.30
4	c1	460	LEU	CA-CB-CG	6.61	130.50	115.30
4	c	414	LEU	CA-CB-CG	6.54	130.33	115.30
5	D1	182	ILE	CG1-CB-CG2	-6.45	97.21	111.40
24	Y	98	LEU	CA-CB-CG	6.40	130.01	115.30
14	o1	101	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A1	199	MET	CA-CB-CG	6.35	124.09	113.30
8	h	41	LEU	CA-CB-CG	6.25	129.66	115.30
11	K1	31	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	338	ASN	C-N-CA	6.06	136.86	121.70
5	d	321	LEU	CA-CB-CG	6.00	129.11	115.30
14	O	223	ASP	CB-CG-OD1	5.98	123.68	118.30
23	S	221	LEU	CA-CB-CG	5.94	128.96	115.30
1	a1	196	PRO	CA-N-CD	-5.86	103.29	111.50
5	d1	162	LEU	CA-CB-CG	5.77	128.57	115.30
5	d	126	MET	CA-CB-CG	5.73	123.04	113.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	123	ILE	CG1-CB-CG2	-5.63	99.00	111.40
4	c	69	MET	CB-CG-SD	5.62	129.26	112.40
27	r1	176	LEU	CA-CB-CG	5.60	128.19	115.30
4	c	69	MET	CA-CB-CG	5.59	122.81	113.30
23	s	280	LEU	CA-CB-CG	5.53	128.01	115.30
5	d	321	LEU	CB-CG-CD2	-5.41	101.81	111.00
5	D	59	TYR	C-N-CA	5.40	135.20	121.70
22	r	221	LEU	CA-CB-CG	5.33	127.56	115.30
1	a	139	MET	C-N-CA	5.31	134.98	121.70
2	B1	341	LEU	CA-CB-CG	5.30	127.50	115.30
11	K	11	LEU	CA-CB-CG	5.30	127.48	115.30
14	O	120	ASP	CB-CG-OD2	5.24	123.02	118.30
21	g	189	ASP	CB-CG-OD1	5.23	123.01	118.30
14	o1	120	ASP	CB-CG-OD2	5.21	122.99	118.30
14	o	120	ASP	CB-CG-OD2	5.21	122.99	118.30
14	O	141	ASP	CB-CG-OD2	5.21	122.99	118.30
14	O1	141	ASP	CB-CG-OD2	5.19	122.97	118.30
14	o1	141	ASP	CB-CG-OD2	5.19	122.97	118.30
14	o	141	ASP	CB-CG-OD2	5.18	122.97	118.30
21	g	131	LEU	CA-CB-CG	5.18	127.22	115.30
14	O1	120	ASP	CB-CG-OD2	5.16	122.94	118.30
14	O1	228	LEU	CA-CB-CG	5.13	127.10	115.30
17	W1	89	LEU	CA-CB-CG	5.12	127.07	115.30
25	u1	109	LEU	CA-CB-CG	5.07	126.97	115.30
24	y1	204	LEU	CA-CB-CG	5.04	126.90	115.30
8	H	30	LEU	CA-CB-CG	5.04	126.89	115.30
8	H	57	PHE	CZ-CE2-CD2	-5.03	114.06	120.10
2	B	50	PRO	CA-CB-CG	-5.00	94.50	104.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/336 (100%)	304 (91%)	30 (9%)	1 (0%)	41	75
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a1	335/336 (100%)	316 (94%)	19 (6%)	0	100	100
2	B	482/484 (100%)	460 (95%)	21 (4%)	1 (0%)	47	79
2	B1	482/484 (100%)	459 (95%)	23 (5%)	0	100	100
2	b	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
2	b1	482/484 (100%)	462 (96%)	20 (4%)	0	100	100
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	V1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	410 (92%)	34 (8%)	3 (1%)	22	61
4	C1	447/449 (100%)	427 (96%)	20 (4%)	0	100	100
4	c	447/449 (100%)	413 (92%)	31 (7%)	3 (1%)	22	61
4	c1	447/449 (100%)	425 (95%)	22 (5%)	0	100	100
5	D	346/348 (99%)	330 (95%)	15 (4%)	1 (0%)	41	75
5	D1	346/348 (99%)	332 (96%)	14 (4%)	0	100	100
5	d	346/348 (99%)	332 (96%)	13 (4%)	1 (0%)	41	75
5	d1	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	E1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
6	e	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
6	e1	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	H1	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
9	i1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
10	j1	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	K1	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	k1	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	4	30
13	m	30/32 (94%)	28 (93%)	1 (3%)	1 (3%)	4	30
14	O	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	34	71
14	O1	236/238 (99%)	214 (91%)	21 (9%)	1 (0%)	34	71
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	34	71
14	o1	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	34	71
15	P	185/187 (99%)	167 (90%)	17 (9%)	1 (0%)	29	67
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	p1	185/187 (99%)	171 (92%)	14 (8%)	0	100	100
16	T	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	3	28
16	T1	28/30 (93%)	27 (96%)	0	1 (4%)	3	28
16	t	28/30 (93%)	27 (96%)	0	1 (4%)	3	28
16	t1	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
17	W1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	Z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
19	z1	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	67
20	N1	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	29	67
20	n	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	17	55
20	n1	218/222 (98%)	198 (91%)	19 (9%)	1 (0%)	29	67
21	G	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	29	67
21	G1	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
21	g	219/221 (99%)	209 (95%)	9 (4%)	1 (0%)	29	67
21	g1	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
22	R	198/202 (98%)	188 (95%)	10 (5%)	0	100	100
22	r	198/202 (98%)	181 (91%)	17 (9%)	0	100	100
23	S	240/243 (99%)	218 (91%)	20 (8%)	2 (1%)	19	58
23	S1	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	13	49
23	s	239/243 (98%)	219 (92%)	18 (8%)	2 (1%)	19	58
23	s1	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	19	58

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	Y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	29	67
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	67
24	y	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	67
24	y1	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	29	67
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	U1	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	25 (100%)	0	0	100	100
25	u1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
26	M1	29/31 (94%)	29 (100%)	0	0	100	100
26	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
27	R1	191/202 (95%)	183 (96%)	8 (4%)	0	100	100
27	r1	191/202 (95%)	181 (95%)	10 (5%)	0	100	100
All	All	14651/14872 (98%)	13772 (94%)	839 (6%)	40 (0%)	44	75

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	257	GLU
4	C	395	VAL
14	O	94	VAL
4	c	257	GLU
4	c	395	VAL
5	d	60	THR
16	t	29	ILE
23	s	92	LYS
14	O1	205	TYR
14	o1	205	TYR
23	s1	284	ASP
5	D	60	THR
15	P	126	SER
16	T	29	ILE
20	N	145	ILE
4	c	173	VAL
14	o	205	TYR
20	n	145	ILE
24	y	146	ILE
4	C	173	VAL
23	S	92	LYS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
24	Y	146	ILE
24	Y1	146	ILE
20	n1	145	ILE
23	s1	92	LYS
24	y1	146	ILE
13	M	3	VAL
21	G	137	ILE
13	m	3	VAL
21	g	137	ILE
20	N1	145	ILE
2	B	401	PHE
1	A	298	ASN
23	s	284	ASP
23	S1	92	LYS
23	S1	284	ASP
23	S	158	VAL
20	n	183	PRO
16	T1	29	ILE
23	S1	158	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	275 (100%)	1 (0%)	91	94
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	387 (100%)	1 (0%)	92	95
2	B1	388/388 (100%)	388 (100%)	0	100	100
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	386 (100%)	2 (0%)	88	93
3	V	25/25 (100%)	25 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
3	v1	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	349 (100%)	1 (0%)	92	95
4	C1	350/350 (100%)	349 (100%)	1 (0%)	92	95
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	348 (99%)	2 (1%)	86	92
5	D	279/279 (100%)	278 (100%)	1 (0%)	91	94
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	278 (100%)	1 (0%)	91	94
5	d1	279/279 (100%)	278 (100%)	1 (0%)	91	94
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	55 (98%)	1 (2%)	59	77
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	33/33 (100%)	33 (100%)	0	100	100
11	K1	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
13	m	27/27 (100%)	27 (100%)	0	100	100
14	O	195/195 (100%)	194 (100%)	1 (0%)	88	93
14	O1	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	194 (100%)	1 (0%)	88	93
14	o1	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	150 (99%)	1 (1%)	84	90
15	P1	151/151 (100%)	150 (99%)	1 (1%)	84	90
15	p	151/151 (100%)	151 (100%)	0	100	100
15	p1	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	33 (97%)	1 (3%)	42	65
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	z	50/50 (100%)	50 (100%)	0	100	100
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	170 (99%)	1 (1%)	86	92
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	86	92
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	167 (99%)	1 (1%)	86	92
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	158/158 (100%)	158 (100%)	0	100	100
22	r	158/158 (100%)	158 (100%)	0	100	100
23	S	189/190 (100%)	188 (100%)	1 (0%)	88	93
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
23	s1	190/190 (100%)	188 (99%)	2 (1%)	73	85
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
25	u1	26/26 (100%)	25 (96%)	1 (4%)	33	59
26	M1	26/26 (100%)	26 (100%)	0	100	100
26	m1	26/26 (100%)	26 (100%)	0	100	100
27	R1	151/157 (96%)	151 (100%)	0	100	100
27	r1	151/157 (96%)	151 (100%)	0	100	100
All	All	11856/11865 (100%)	11832 (100%)	24 (0%)	93	96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	476	ARG
4	C	406	ASN
5	D	180	ARG
14	O	124	ARG
15	P	147	ARG
17	W	65	MET
20	N	83	LYS
21	G	87	ARG
23	S	285	ARG
1	a	108	ASN
5	d	180	ARG
14	o	124	ARG
20	n	170	ASN
4	C1	406	ASN
15	P1	228	LYS
2	b1	224	ARG
2	b1	418	LYS
4	c1	384	MET
4	c1	406	ASN
5	d1	180	ARG
8	h1	79	ASN
23	s1	99	LYS
23	s1	132	LYS
25	u1	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	73	GLN
4	C	147	ASN
4	C	315	ASN
4	C	403	ASN
6	E	61	GLN
14	O	82	ASN
1	a	298	ASN
1	a	303	ASN
1	a	332	HIS
2	b	425	GLN
5	d	220	ASN
11	k	40	GLN
14	o	238	GLN
15	p	129	GLN
20	n	146	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
21	g	133	ASN
23	s	281	GLN
1	A1	234	ASN
1	A1	338	ASN
2	B1	285	GLN
5	D1	186	GLN
5	D1	322	ASN
5	D1	350	ASN
14	O1	82	ASN
15	P1	109	ASN
17	W1	66	ASN
24	Y1	158	GLN
24	Y1	248	ASN
1	a1	26	ASN
1	a1	181	ASN
1	a1	187	GLN
2	b1	194	ASN
3	v1	8	GLN
4	c1	152	HIS
4	c1	406	ASN
4	c1	429	HIS
5	d1	292	ASN
5	d1	336	HIS
15	p1	203	GLN
21	g1	239	ASN
24	y1	142	ASN
24	y1	144	ASN
24	y1	149	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	SEP	r1	84	27	8,9,10	1.55	1 (12%)	8,12,14	1.26	1 (12%)
27	SEP	R1	84	27	8,9,10	1.56	1 (12%)	8,12,14	1.86	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SEP	r1	84	27	-	3/5/8/10	-
27	SEP	R1	84	27	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	r1	84	SEP	P-O1P	3.40	1.61	1.50
27	R1	84	SEP	P-O1P	3.37	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R1	84	SEP	OG-CB-CA	3.54	111.59	108.14
27	R1	84	SEP	P-OG-CB	-3.40	108.92	118.30
27	r1	84	SEP	P-OG-CB	-2.20	112.25	118.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	R1	84	SEP	CB-OG-P-O1P
27	R1	84	SEP	CB-OG-P-O2P
27	R1	84	SEP	CB-OG-P-O3P
27	r1	84	SEP	CB-OG-P-O2P
27	r1	84	SEP	CB-OG-P-O1P
27	r1	84	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 703 ligands modelled in this entry, 16 are monoatomic - leaving 687 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
35	LMG	h	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.10	2 (3%)
31	CLA	b	614	-	65,73,73	1.32	6 (9%)	76,113,113	1.96	18 (23%)
47	CHL	n1	605	-	66,74,74	0.82	3 (4%)	73,114,114	1.22	12 (16%)
31	CLA	C1	504	-	65,73,73	1.34	7 (10%)	76,113,113	2.06	15 (19%)
31	CLA	b1	607	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
41	LHG	C1	525	-	46,46,48	0.40	0	49,52,54	1.11	2 (4%)
45	HEM	F1	101	6	41,50,50	1.47	5 (12%)	45,82,82	1.29	4 (8%)
47	CHL	Y	605	24	46,54,74	1.00	2 (4%)	49,90,114	1.45	9 (18%)
48	LUT	S1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
31	CLA	N	604	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	20 (26%)
48	LUT	G1	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.05	10 (19%)
31	CLA	c1	502	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	19 (25%)
34	SQD	b1	626	-	53,54,54	0.80	0	62,65,65	0.90	2 (3%)
49	XAT	y	622	-	39,47,47	0.67	1 (2%)	54,74,74	3.73	19 (35%)
57	PTY	y1	627	-	18,18,49	1.30	3 (16%)	21,23,54	1.42	2 (9%)
31	CLA	c	508	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	15 (19%)
32	PHO	a	409	-	51,69,69	1.02	4 (7%)	47,99,99	1.23	5 (10%)
41	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.07	4 (8%)
41	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.05	3 (5%)
31	CLA	n	614	-	49,57,73	1.55	9 (18%)	55,93,113	2.26	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	n1	602	-	65,73,73	1.33	7 (10%)	76,113,113	2.03	18 (23%)
38	DGA	J1	101	-	28,28,43	1.30	3 (10%)	30,30,45	1.26	2 (6%)
31	CLA	B1	603	-	65,73,73	1.35	9 (13%)	76,113,113	2.00	18 (23%)
31	CLA	S	617	-	50,58,73	1.54	8 (16%)	58,95,113	2.24	17 (29%)
35	LMG	d1	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.17	2 (3%)
31	CLA	n1	604	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	18 (23%)
31	CLA	r1	602	-	60,68,73	1.41	9 (15%)	70,107,113	2.07	21 (30%)
48	LUT	s1	621	-	42,43,43	2.33	1 (2%)	51,60,60	2.08	14 (27%)
31	CLA	Y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	17 (22%)
31	CLA	d1	403	-	65,73,73	1.35	8 (12%)	76,113,113	2.06	18 (23%)
31	CLA	B1	609	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	18 (23%)
31	CLA	A1	406	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	18 (23%)
31	CLA	c1	505	-	65,73,73	1.39	9 (13%)	76,113,113	1.92	15 (19%)
31	CLA	s1	610	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	16 (21%)
33	BCR	c1	516	-	41,41,41	1.85	4 (9%)	56,56,56	4.44	16 (28%)
35	LMG	c1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
47	CHL	Y	601	-	66,74,74	0.83	2 (3%)	73,114,114	1.20	10 (13%)
49	XAT	g1	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.80	13 (24%)
47	CHL	n	605	-	66,74,74	0.86	3 (4%)	73,114,114	1.22	12 (16%)
47	CHL	g	601	21	66,74,74	0.84	3 (4%)	73,114,114	1.28	12 (16%)
40	DGD	c	519	-	63,63,67	1.10	6 (9%)	77,77,81	1.04	3 (3%)
34	SQD	A1	412	-	50,51,54	0.82	0	59,62,65	0.93	3 (5%)
52	3PH	S1	626	-	47,47,47	0.85	4 (8%)	51,52,52	4.44	4 (7%)
31	CLA	r1	608	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	15 (21%)
33	BCR	C1	517	-	41,41,41	1.91	4 (9%)	56,56,56	4.60	18 (32%)
31	CLA	c1	507	-	65,73,73	1.38	9 (13%)	76,113,113	1.93	18 (23%)
47	CHL	n1	606	-	66,74,74	0.85	3 (4%)	73,114,114	1.17	9 (12%)
31	CLA	a	407	-	49,57,73	1.57	8 (16%)	55,93,113	2.23	17 (30%)
31	CLA	c	502	-	65,73,73	1.33	7 (10%)	76,113,113	2.07	18 (23%)
31	CLA	C1	506	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	18 (23%)
33	BCR	c	515	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	18 (32%)
43	BCT	D1	401	-	2,3,3	1.24	0	2,3,3	4.24	2 (100%)
35	LMG	c	521	-	51,51,55	1.08	5 (9%)	59,59,63	1.19	3 (5%)
47	CHL	y1	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.22	10 (13%)
31	CLA	A	406	-	65,73,73	1.32	6 (9%)	76,113,113	2.08	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	CHL	Y	606	-	66,74,74	0.84	3 (4%)	73,114,114	1.20	11 (15%)
31	CLA	G	611	-	45,53,73	1.64	9 (20%)	52,89,113	2.22	16 (30%)
31	CLA	N1	610	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	13 (17%)
47	CHL	Y1	601	24	66,74,74	0.83	2 (3%)	73,114,114	1.13	7 (9%)
33	BCR	c	517	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	15 (26%)
33	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.22	12 (21%)
34	SQD	c1	526	-	53,54,54	0.79	0	62,65,65	0.90	3 (4%)
33	BCR	d	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.14	17 (30%)
31	CLA	a1	405	-	65,73,73	1.33	6 (9%)	76,113,113	2.10	21 (27%)
31	CLA	R	612	-	60,68,73	1.42	8 (13%)	70,107,113	2.03	18 (25%)
48	LUT	S	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.06	15 (29%)
35	LMG	c1	521	-	51,51,55	1.07	6 (11%)	59,59,63	1.13	3 (5%)
31	CLA	S	610	-	65,73,73	1.39	9 (13%)	76,113,113	1.93	17 (22%)
47	CHL	Y1	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.29	12 (16%)
31	CLA	R1	602	-	60,68,73	1.40	8 (13%)	70,107,113	2.13	18 (25%)
31	CLA	Y	608	-	50,58,73	1.56	9 (18%)	58,95,113	2.20	16 (27%)
47	CHL	N	601	20	66,74,74	0.84	3 (4%)	73,114,114	1.20	9 (12%)
50	NEX	Y	623	-	38,46,46	3.29	9 (23%)	50,70,70	2.05	15 (30%)
41	LHG	D1	409	-	48,48,48	0.39	0	51,54,54	1.10	5 (9%)
35	LMG	A1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.16	4 (7%)
31	CLA	b1	605	-	65,73,73	1.34	6 (9%)	76,113,113	2.26	19 (25%)
47	CHL	G	606	-	50,58,74	0.99	3 (6%)	52,94,114	1.38	9 (17%)
37	C7Z	b	620	-	43,43,43	5.42	26 (60%)	58,60,60	2.17	18 (31%)
31	CLA	c1	510	-	65,73,73	1.35	6 (9%)	76,113,113	1.96	15 (19%)
47	CHL	R1	607	-	50,58,74	0.94	2 (4%)	52,94,114	1.39	10 (19%)
31	CLA	s1	611	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	19 (25%)
47	CHL	r1	607	-	50,58,74	0.95	2 (4%)	52,94,114	1.34	9 (17%)
31	CLA	S1	614	-	55,63,73	1.47	7 (12%)	64,101,113	2.10	16 (25%)
31	CLA	G1	610	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	18 (23%)
31	CLA	C1	503	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	17 (22%)
31	CLA	c1	506	-	65,73,73	1.35	7 (10%)	76,113,113	1.94	15 (19%)
38	DGA	b	623	-	43,43,43	1.13	2 (4%)	45,45,45	1.52	3 (6%)
54	4RF	k1	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.90	3 (5%)
38	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.50	3 (6%)
31	CLA	g1	611	-	65,73,73	1.35	9 (13%)	76,113,113	1.98	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	g1	603	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	18 (23%)
31	CLA	b	602	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	17 (22%)
47	CHL	g	605	-	48,56,74	0.95	2 (4%)	51,92,114	1.39	11 (21%)
31	CLA	S1	613	-	55,63,73	1.48	8 (14%)	64,101,113	2.13	14 (21%)
31	CLA	Y1	608	-	50,58,73	1.56	10 (20%)	58,95,113	2.23	16 (27%)
34	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
47	CHL	Y1	609	-	66,74,74	0.85	3 (4%)	73,114,114	1.28	13 (17%)
31	CLA	y1	602	-	65,73,73	1.33	7 (10%)	76,113,113	2.03	17 (22%)
48	LUT	N1	620	-	42,43,43	2.40	1 (2%)	51,60,60	1.89	10 (19%)
56	ERG	R1	626	-	31,32,32	7.76	19 (61%)	47,50,50	2.68	20 (42%)
31	CLA	b	608	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	17 (22%)
31	CLA	d	403	-	65,73,73	1.38	7 (10%)	76,113,113	1.99	15 (19%)
47	CHL	y	605	24	46,54,74	0.98	2 (4%)	49,90,114	1.37	11 (22%)
57	PTY	Y1	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.39	2 (9%)
40	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.01	3 (4%)
41	LHG	S1	624	-	44,44,48	0.41	0	47,50,54	1.11	4 (8%)
50	NEX	R	622	-	38,46,46	3.32	12 (31%)	50,70,70	1.89	11 (22%)
31	CLA	B1	615	-	65,73,73	1.37	10 (15%)	76,113,113	1.96	15 (19%)
55	LMT	R1	625	-	36,36,36	1.16	5 (13%)	47,47,47	1.00	2 (4%)
50	NEX	N	623	-	38,46,46	3.39	9 (23%)	50,70,70	1.81	13 (26%)
47	CHL	n	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.28	9 (12%)
31	CLA	A1	410	-	60,68,73	1.39	8 (13%)	70,107,113	2.16	20 (28%)
31	CLA	N1	613	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	17 (22%)
47	CHL	N1	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.21	11 (15%)
47	CHL	G1	605	-	48,56,74	0.94	2 (4%)	51,92,114	1.37	9 (17%)
31	CLA	S	611	-	65,73,73	1.38	8 (12%)	76,113,113	1.95	16 (21%)
31	CLA	S1	602	-	60,68,73	1.40	8 (13%)	70,107,113	2.10	20 (28%)
31	CLA	c1	512	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	18 (23%)
31	CLA	S1	612	-	45,53,73	1.60	7 (15%)	52,89,113	2.22	14 (26%)
47	CHL	G	608	-	44,52,74	1.01	3 (6%)	46,87,114	1.46	9 (19%)
47	CHL	S1	601	23	46,54,74	1.01	3 (6%)	49,90,114	1.37	7 (14%)
31	CLA	N	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
41	LHG	n	624	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
33	BCR	a	411	-	41,41,41	1.85	4 (9%)	56,56,56	4.32	15 (26%)
48	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.14	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	A1	405	-	65,73,73	1.40	8 (12%)	76,113,113	2.15	23 (30%)
33	BCR	C1	514	-	41,41,41	1.86	4 (9%)	56,56,56	4.45	17 (30%)
48	LUT	G1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.14	12 (23%)
40	DGD	C	519	-	63,63,67	1.12	6 (9%)	77,77,81	1.09	5 (6%)
41	LHG	d1	410	-	38,38,48	0.42	0	41,44,54	1.16	3 (7%)
50	NEX	R1	622	-	38,46,46	3.29	9 (23%)	50,70,70	1.82	11 (22%)
47	CHL	r	606	-	44,52,74	1.04	3 (6%)	46,87,114	1.32	7 (15%)
31	CLA	S	614	-	55,63,73	1.46	7 (12%)	64,101,113	2.09	14 (21%)
31	CLA	B	612	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	15 (19%)
49	XAT	N1	622	-	39,47,47	0.68	1 (2%)	54,74,74	2.01	14 (25%)
33	BCR	A1	411	-	41,41,41	1.82	4 (9%)	56,56,56	4.39	15 (26%)
31	CLA	Y1	614	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	18 (23%)
57	PTY	y1	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.06	2 (3%)
31	CLA	s	611	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
31	CLA	s	603	-	65,73,73	1.37	9 (13%)	76,113,113	1.91	15 (19%)
53	SPH	Y	625	-	19,20,20	0.62	0	18,21,21	1.13	1 (5%)
31	CLA	s1	613	-	55,63,73	1.50	9 (16%)	64,101,113	2.13	15 (23%)
31	CLA	n	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.09	18 (23%)
32	PHO	A	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.15	5 (10%)
31	CLA	B1	605	-	65,73,73	1.32	7 (10%)	76,113,113	2.10	19 (25%)
31	CLA	C	503	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	17 (22%)
47	CHL	S1	608	-	61,69,74	0.88	3 (4%)	67,108,114	1.33	11 (16%)
41	LHG	y1	624	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
31	CLA	n	611	-	49,57,73	1.59	9 (18%)	55,93,113	2.31	16 (29%)
35	LMG	C1	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.11	4 (6%)
35	LMG	B	622	-	44,44,55	0.87	2 (4%)	52,52,63	1.02	2 (3%)
31	CLA	N	610	-	65,73,73	1.39	8 (12%)	76,113,113	2.02	19 (25%)
33	BCR	C	515	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	16 (28%)
47	CHL	Y1	606	-	66,74,74	0.86	3 (4%)	73,114,114	1.16	7 (9%)
31	CLA	g	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.00	17 (22%)
33	BCR	D	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.21	18 (32%)
37	C7Z	B1	620	-	43,43,43	5.36	26 (60%)	58,60,60	2.40	21 (36%)
31	CLA	G	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.12	22 (28%)
31	CLA	c	512	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	19 (25%)
50	NEX	S1	623	-	38,46,46	3.31	10 (26%)	50,70,70	1.84	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	LUT	g	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.09	12 (23%)
41	LHG	Y1	624	-	48,48,48	0.39	0	51,54,54	1.00	3 (5%)
31	CLA	r	603	-	60,68,73	1.42	9 (15%)	70,107,113	1.99	15 (21%)
31	CLA	R1	612	-	60,68,73	1.42	10 (16%)	70,107,113	2.07	17 (24%)
47	CHL	G	601	-	66,74,74	0.91	4 (6%)	73,114,114	1.21	10 (13%)
47	CHL	n	606	-	66,74,74	0.87	4 (6%)	73,114,114	1.21	10 (13%)
47	CHL	g	606	-	50,58,74	0.88	2 (4%)	52,94,114	1.52	10 (19%)
48	LUT	g1	621	-	42,43,43	2.38	1 (2%)	51,60,60	1.90	12 (23%)
47	CHL	S1	607	-	43,51,74	1.01	3 (6%)	45,86,114	1.47	10 (22%)
31	CLA	B1	612	-	65,73,73	1.33	6 (9%)	76,113,113	1.99	16 (21%)
31	CLA	y	612	-	65,73,73	1.37	7 (10%)	76,113,113	1.95	14 (18%)
31	CLA	C	508	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	18 (23%)
31	CLA	S	613	-	55,63,73	1.49	8 (14%)	64,101,113	2.34	18 (28%)
31	CLA	y1	614	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	17 (22%)
31	CLA	G1	613	-	65,73,73	1.35	9 (13%)	76,113,113	2.03	15 (19%)
31	CLA	s	609	-	60,68,73	1.43	10 (16%)	70,107,113	2.01	16 (22%)
31	CLA	B	615	-	65,73,73	1.34	7 (10%)	76,113,113	2.18	19 (25%)
53	SPH	y1	625	-	19,20,20	0.64	0	18,21,21	1.05	0
31	CLA	B	617	-	65,73,73	1.37	7 (10%)	76,113,113	4.32	18 (23%)
31	CLA	s1	604	-	55,63,73	1.49	10 (18%)	64,101,113	2.17	17 (26%)
31	CLA	c	513	-	65,73,73	1.39	9 (13%)	76,113,113	1.94	15 (19%)
47	CHL	N1	601	20	66,74,74	0.84	3 (4%)	73,114,114	1.27	12 (16%)
51	LPX	S	625	-	29,29,29	1.01	2 (6%)	31,33,33	0.96	1 (3%)
41	LHG	d	410	-	38,38,48	0.42	0	41,44,54	1.17	3 (7%)
39	GOL	B	627	-	5,5,5	0.56	0	5,5,5	0.26	0
31	CLA	Y1	604	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	21 (27%)
31	CLA	n	604	-	65,73,73	1.32	6 (9%)	76,113,113	2.14	21 (27%)
41	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
31	CLA	G1	614	-	49,57,73	1.56	9 (18%)	55,93,113	2.26	15 (27%)
41	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.02	3 (6%)
47	CHL	R1	606	-	44,52,74	1.04	2 (4%)	46,87,114	1.27	5 (10%)
50	NEX	G1	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.87	14 (28%)
33	BCR	d1	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	18 (32%)
47	CHL	Y	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.24	10 (13%)
34	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMG	J	101	-	45,45,55	0.91	3 (6%)	53,53,63	1.08	3 (5%)
31	CLA	c	507	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	18 (23%)
35	LMG	d	411	-	46,46,55	0.91	3 (6%)	54,54,63	1.20	3 (5%)
34	SQD	C1	526	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
54	4RF	I1	102	-	56,56,56	1.07	3 (5%)	59,59,59	0.95	3 (5%)
52	3PH	i	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.18	2 (3%)
31	CLA	g	604	-	49,57,73	1.57	8 (16%)	55,93,113	2.31	19 (34%)
47	CHL	G1	601	21	66,74,74	0.83	3 (4%)	73,114,114	1.30	14 (19%)
31	CLA	N	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	17 (22%)
47	CHL	Y1	605	24	46,54,74	0.98	3 (6%)	49,90,114	1.39	9 (18%)
52	3PH	T1	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.10	2 (3%)
34	SQD	B1	626	-	53,54,54	0.80	0	62,65,65	0.91	2 (3%)
41	LHG	L	101	-	48,48,48	0.40	0	51,54,54	0.96	2 (3%)
31	CLA	R	608	-	60,68,73	1.43	10 (16%)	70,107,113	2.01	14 (20%)
31	CLA	A	410	-	60,68,73	1.43	10 (16%)	70,107,113	2.13	19 (27%)
47	CHL	G1	607	-	66,74,74	0.80	2 (3%)	73,114,114	1.18	9 (12%)
31	CLA	G	612	-	43,51,73	1.68	8 (18%)	49,86,113	2.22	13 (26%)
52	3PH	B1	624	-	47,47,47	0.86	3 (6%)	51,52,52	1.11	2 (3%)
31	CLA	s	610	-	65,73,73	1.38	9 (13%)	76,113,113	2.02	17 (22%)
48	LUT	S	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.05	13 (25%)
55	LMT	r1	625	-	36,36,36	1.18	5 (13%)	47,47,47	0.99	2 (4%)
31	CLA	d	402	-	65,73,73	1.37	8 (12%)	76,113,113	1.88	16 (21%)
42	LMK	c	627	-	38,39,53	1.47	2 (5%)	41,46,60	1.36	2 (4%)
31	CLA	Y1	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	19 (25%)
47	CHL	N1	609	-	66,74,74	0.81	2 (3%)	73,114,114	1.17	9 (12%)
31	CLA	G1	604	-	49,57,73	1.56	9 (18%)	55,93,113	2.22	18 (32%)
31	CLA	y	603	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	18 (23%)
31	CLA	G1	612	-	43,51,73	1.68	9 (20%)	49,86,113	2.18	13 (26%)
34	SQD	B	621	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
31	CLA	B	616	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	18 (23%)
48	LUT	R1	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.14	14 (27%)
49	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.73	17 (31%)
47	CHL	g1	609	-	66,74,74	0.85	2 (3%)	73,114,114	1.14	10 (13%)
31	CLA	y1	612	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	16 (21%)
31	CLA	C1	507	-	65,73,73	1.34	8 (12%)	76,113,113	2.04	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	B1	606	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	16 (21%)
49	XAT	n	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.94	11 (20%)
35	LMG	H1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.09	2 (3%)
32	PHO	A1	409	-	51,69,69	0.99	4 (7%)	47,99,99	1.29	5 (10%)
31	CLA	b1	602	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	16 (21%)
47	CHL	y	609	-	66,74,74	0.84	3 (4%)	73,114,114	1.18	10 (13%)
41	LHG	s1	624	-	44,44,48	0.41	0	47,50,54	1.02	3 (6%)
31	CLA	S1	609	-	60,68,73	1.41	10 (16%)	70,107,113	2.09	18 (25%)
41	LHG	d1	409	-	48,48,48	0.41	0	51,54,54	0.98	2 (3%)
31	CLA	r	604	-	49,57,73	1.53	8 (16%)	55,93,113	2.28	15 (27%)
48	LUT	s	621	-	42,43,43	2.33	1 (2%)	51,60,60	1.91	14 (27%)
31	CLA	g	602	-	65,73,73	1.31	8 (12%)	76,113,113	2.05	19 (25%)
31	CLA	C1	505	-	65,73,73	1.35	8 (12%)	76,113,113	2.01	16 (21%)
41	LHG	g1	624	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
57	PTY	Y1	626	-	49,49,49	0.87	3 (6%)	52,54,54	1.05	2 (3%)
31	CLA	a1	406	-	65,73,73	1.32	8 (12%)	76,113,113	2.05	17 (22%)
47	CHL	N	609	-	66,74,74	0.80	2 (3%)	73,114,114	1.23	11 (15%)
31	CLA	b1	604	-	65,73,73	1.33	8 (12%)	76,113,113	2.01	18 (23%)
31	CLA	N1	614	-	49,57,73	1.55	9 (18%)	55,93,113	2.33	17 (30%)
48	LUT	n1	621	-	42,43,43	2.40	1 (2%)	51,60,60	2.19	16 (31%)
31	CLA	n	612	-	45,53,73	1.63	7 (15%)	52,89,113	2.06	17 (32%)
39	GOL	y	626	-	5,5,5	0.53	0	5,5,5	0.33	0
40	DGD	C1	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.98	3 (4%)
31	CLA	r	608	-	60,68,73	1.41	8 (13%)	70,107,113	2.04	14 (20%)
47	CHL	n	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.37	8 (15%)
31	CLA	c1	509	-	65,73,73	1.34	6 (9%)	76,113,113	1.94	16 (21%)
33	BCR	D1	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	16 (28%)
31	CLA	b	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.12	18 (23%)
38	DGA	j1	101	-	28,28,43	1.29	3 (10%)	30,30,45	1.30	2 (6%)
31	CLA	A1	407	-	50,58,73	1.53	8 (16%)	58,95,113	2.27	20 (34%)
33	BCR	b1	618	-	41,41,41	1.86	4 (9%)	56,56,56	4.49	20 (35%)
31	CLA	r1	610	-	60,68,73	1.42	8 (13%)	70,107,113	2.00	17 (24%)
38	DGA	c1	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
45	HEM	f1	101	-	41,50,50	1.46	4 (9%)	45,82,82	1.41	5 (11%)
44	PL9	d	405	-	55,55,55	1.26	6 (10%)	68,69,69	1.50	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	G1	611	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	17 (22%)
31	CLA	b1	616	-	65,73,73	1.38	8 (12%)	76,113,113	1.92	15 (19%)
31	CLA	b	617	-	65,73,73	1.35	7 (10%)	76,113,113	4.30	17 (22%)
38	DGA	C1	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.51	3 (6%)
41	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
44	PL9	D	405	-	55,55,55	1.27	4 (7%)	68,69,69	1.56	13 (19%)
31	CLA	n1	611	-	49,57,73	1.56	9 (18%)	55,93,113	2.26	15 (27%)
41	LHG	D	410	-	38,38,48	0.44	0	41,44,54	1.03	2 (4%)
31	CLA	s1	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.08	17 (22%)
48	LUT	N	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.06	12 (23%)
49	XAT	r	622	-	39,47,47	0.68	1 (2%)	54,74,74	2.15	17 (31%)
31	CLA	c1	513	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	21 (27%)
31	CLA	G	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.09	20 (26%)
31	CLA	c1	511	-	65,73,73	1.35	8 (12%)	76,113,113	2.16	21 (27%)
31	CLA	S1	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.10	19 (25%)
50	NEX	y	623	-	38,46,46	3.22	9 (23%)	50,70,70	1.93	15 (30%)
31	CLA	N1	602	-	65,73,73	1.30	7 (10%)	76,113,113	2.02	19 (25%)
41	LHG	y	624	-	48,48,48	0.38	0	51,54,54	1.08	3 (5%)
31	CLA	C1	501	-	65,73,73	1.36	9 (13%)	76,113,113	2.00	18 (23%)
31	CLA	G	610	-	65,73,73	1.34	8 (12%)	76,113,113	2.07	18 (23%)
40	DGD	B1	623	-	44,44,67	0.84	1 (2%)	58,58,81	1.26	5 (8%)
31	CLA	Y	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.03	18 (23%)
31	CLA	C	504	-	65,73,73	1.32	8 (12%)	76,113,113	2.09	18 (23%)
50	NEX	s1	623	-	38,46,46	3.43	12 (31%)	50,70,70	1.81	10 (20%)
31	CLA	c1	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	18 (23%)
47	CHL	s1	601	23	46,54,74	0.98	2 (4%)	49,90,114	1.28	7 (14%)
31	CLA	B1	604	-	65,73,73	1.38	9 (13%)	76,113,113	1.90	16 (21%)
52	3PH	b1	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.16	2 (3%)
31	CLA	B	614	-	65,73,73	1.33	6 (9%)	76,113,113	1.96	17 (22%)
47	CHL	N	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.33	11 (15%)
47	CHL	g	607	-	50,58,74	0.87	2 (4%)	52,94,114	1.40	11 (21%)
47	CHL	y	601	24	66,74,74	0.81	2 (3%)	73,114,114	1.17	11 (15%)
31	CLA	B	605	-	65,73,73	1.36	8 (12%)	76,113,113	2.14	17 (22%)
31	CLA	c	505	-	65,73,73	1.37	9 (13%)	76,113,113	1.97	15 (19%)
39	GOL	b	624	-	5,5,5	0.58	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	D	403	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	19 (25%)
33	BCR	c	516	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	20 (35%)
47	CHL	g1	601	-	66,74,74	0.83	3 (4%)	73,114,114	1.21	9 (12%)
31	CLA	s1	612	-	45,53,73	1.58	6 (13%)	52,89,113	2.31	17 (32%)
31	CLA	B	606	-	65,73,73	1.35	9 (13%)	76,113,113	1.99	17 (22%)
50	NEX	g1	623	-	38,46,46	3.37	10 (26%)	50,70,70	2.07	13 (26%)
31	CLA	N1	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	17 (22%)
31	CLA	G1	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	17 (22%)
41	LHG	N	624	-	48,48,48	0.37	0	51,54,54	1.16	3 (5%)
31	CLA	c	504	-	65,73,73	1.31	6 (9%)	76,113,113	2.20	20 (26%)
34	SQD	B1	621	-	41,42,54	0.87	0	50,53,65	0.95	3 (6%)
47	CHL	y	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.25	9 (12%)
41	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.13	3 (6%)
31	CLA	g1	612	-	43,51,73	1.67	8 (18%)	49,86,113	2.21	13 (26%)
47	CHL	N1	606	-	66,74,74	0.86	3 (4%)	73,114,114	1.22	12 (16%)
31	CLA	S	603	-	65,73,73	1.37	10 (15%)	76,113,113	1.90	13 (17%)
34	SQD	b	621	-	53,54,54	0.80	0	62,65,65	0.89	2 (3%)
35	LMG	a	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.20	4 (7%)
48	LUT	G	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.99	12 (23%)
31	CLA	G	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	19 (25%)
31	CLA	A	405	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
31	CLA	S	609	-	60,68,73	1.42	10 (16%)	70,107,113	1.99	18 (25%)
47	CHL	N1	605	20	66,74,74	0.85	2 (3%)	73,114,114	1.25	11 (15%)
31	CLA	b	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.94	15 (19%)
35	LMG	H	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.08	2 (3%)
48	LUT	y1	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.96	9 (17%)
31	CLA	B1	608	-	65,73,73	1.36	7 (10%)	76,113,113	2.03	16 (21%)
31	CLA	C1	511	-	65,73,73	1.34	6 (9%)	76,113,113	2.00	18 (23%)
31	CLA	b	611	-	65,73,73	1.36	9 (13%)	76,113,113	2.02	18 (23%)
47	CHL	s	606	-	44,52,74	1.02	3 (6%)	46,87,114	1.42	9 (19%)
48	LUT	y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.08	13 (25%)
41	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.03	4 (8%)
31	CLA	c	501	-	65,73,73	1.35	9 (13%)	76,113,113	2.01	17 (22%)
47	CHL	g1	606	-	50,58,74	0.99	3 (6%)	52,94,114	1.40	11 (21%)
40	DGD	C1	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.93	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
41	LHG	s	624	-	44,44,48	0.41	0	47,50,54	1.11	3 (6%)
47	CHL	n1	608	-	50,58,74	0.89	2 (4%)	52,94,114	1.42	10 (19%)
47	CHL	G1	606	-	50,58,74	0.95	3 (6%)	52,94,114	1.38	8 (15%)
38	DGA	b1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.47	3 (6%)
49	XAT	r1	621	-	39,47,47	0.67	1 (2%)	54,74,74	1.92	16 (29%)
31	CLA	B	608	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	17 (22%)
31	CLA	r	610	-	60,68,73	1.42	9 (15%)	70,107,113	2.05	19 (27%)
51	LPX	s1	625	-	29,29,29	1.03	2 (6%)	31,33,33	0.96	1 (3%)
28	OEX	A	401	1,4	0,15,15	-	-	-	-	-
31	CLA	Y	613	-	65,73,73	1.35	7 (10%)	76,113,113	2.03	18 (23%)
43	BCT	d	401	29	2,3,3	1.26	0	2,3,3	4.15	2 (100%)
46	RRX	H1	101	-	42,42,42	4.85	24 (57%)	57,58,58	2.65	21 (36%)
31	CLA	s	612	-	45,53,73	1.62	8 (17%)	52,89,113	2.21	15 (28%)
31	CLA	a1	407	-	49,57,73	1.53	7 (14%)	55,93,113	2.35	19 (34%)
31	CLA	N1	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.07	19 (25%)
43	BCT	d1	401	-	2,3,3	1.16	0	2,3,3	4.35	2 (100%)
40	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	0.97	2 (2%)
47	CHL	s	601	23	46,54,74	1.02	4 (8%)	49,90,114	1.40	7 (14%)
50	NEX	n1	623	-	38,46,46	3.28	10 (26%)	50,70,70	1.78	13 (26%)
31	CLA	S	612	-	45,53,73	1.63	8 (17%)	52,89,113	2.14	13 (25%)
31	CLA	b1	617	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	16 (21%)
40	DGD	c	523	-	67,67,67	1.17	7 (10%)	81,81,81	0.95	2 (2%)
54	4RF	K1	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.85	3 (5%)
40	DGD	c1	518	-	56,56,67	1.01	4 (7%)	70,70,81	0.97	3 (4%)
46	RRX	h	101	-	42,42,42	4.90	24 (57%)	57,58,58	1.94	17 (29%)
35	LMG	b1	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.16	3 (5%)
31	CLA	r1	604	-	49,57,73	1.54	8 (16%)	55,93,113	2.31	16 (29%)
31	CLA	B1	611	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	18 (23%)
47	CHL	N	606	-	66,74,74	0.89	3 (4%)	73,114,114	1.20	9 (12%)
47	CHL	G	607	-	50,58,74	0.89	2 (4%)	52,94,114	1.45	10 (19%)
53	SPH	A1	414	-	19,20,20	0.67	0	18,21,21	0.92	0
52	3PH	S	626	-	47,47,47	0.87	4 (8%)	51,52,52	1.10	2 (3%)
31	CLA	G1	603	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	16 (21%)
31	CLA	b	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	19 (25%)
31	CLA	R1	610	-	60,68,73	1.38	7 (11%)	70,107,113	2.05	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	s1	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	17 (24%)
31	CLA	D1	402	-	65,73,73	1.37	7 (10%)	76,113,113	1.94	14 (18%)
31	CLA	a	410	-	60,68,73	1.41	8 (13%)	70,107,113	2.13	17 (24%)
31	CLA	N	612	-	45,53,73	1.64	8 (17%)	52,89,113	2.13	12 (23%)
31	CLA	B1	616	-	65,73,73	1.35	7 (10%)	76,113,113	1.94	16 (21%)
33	BCR	b1	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.37	16 (28%)
48	LUT	r	620	-	42,43,43	2.36	1 (2%)	51,60,60	2.12	13 (25%)
31	CLA	B	603	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	19 (25%)
31	CLA	B1	614	-	65,73,73	1.33	7 (10%)	76,113,113	1.93	18 (23%)
31	CLA	b	609	-	65,73,73	1.41	9 (13%)	76,113,113	2.09	18 (23%)
47	CHL	r	607	-	50,58,74	0.95	3 (6%)	52,94,114	1.38	8 (15%)
41	LHG	D1	410	-	38,38,48	0.42	0	41,44,54	1.09	3 (7%)
31	CLA	D1	403	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
34	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
47	CHL	G1	609	-	66,74,74	0.84	2 (3%)	73,114,114	1.17	10 (13%)
32	PHO	A	409	-	51,69,69	1.00	4 (7%)	47,99,99	1.22	4 (8%)
50	NEX	s	623	-	38,46,46	3.33	12 (31%)	50,70,70	1.81	12 (24%)
51	LPX	s	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.96	1 (3%)
31	CLA	S	605	-	50,58,73	1.54	8 (16%)	58,95,113	2.38	19 (32%)
31	CLA	G	614	-	49,57,73	1.54	7 (14%)	55,93,113	2.30	18 (32%)
31	CLA	C	505	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	16 (21%)
31	CLA	B1	607	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	17 (22%)
44	PL9	d1	405	-	55,55,55	1.07	2 (3%)	68,69,69	1.57	12 (17%)
53	SPH	y	625	-	19,20,20	0.64	0	18,21,21	1.13	2 (11%)
41	LHG	d	409	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
47	CHL	g	609	-	66,74,74	0.87	3 (4%)	73,114,114	1.16	10 (13%)
31	CLA	b1	608	-	65,73,73	1.34	6 (9%)	76,113,113	2.02	19 (25%)
31	CLA	n1	612	-	45,53,73	1.64	9 (20%)	52,89,113	2.09	14 (26%)
31	CLA	S1	617	23	50,58,73	1.54	8 (16%)	58,95,113	2.26	16 (27%)
31	CLA	y	602	-	65,73,73	1.32	8 (12%)	76,113,113	2.12	20 (26%)
47	CHL	y1	601	24	66,74,74	0.82	2 (3%)	73,114,114	1.17	8 (10%)
28	OEX	a1	401	1,4	0,15,15	-	-	-	-	-
48	LUT	s1	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.05	14 (27%)
31	CLA	s1	602	-	60,68,73	1.39	8 (13%)	70,107,113	2.03	21 (30%)
33	BCR	a1	411	-	41,41,41	1.85	4 (9%)	56,56,56	4.43	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	BCR	A	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	13 (23%)
41	LHG	S	624	-	44,44,48	0.41	0	47,50,54	1.13	3 (6%)
33	BCR	c	514	-	41,41,41	1.88	4 (9%)	56,56,56	4.51	19 (33%)
31	CLA	b	604	-	65,73,73	1.37	9 (13%)	76,113,113	1.91	16 (21%)
33	BCR	C	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.39	12 (21%)
50	NEX	S	622	-	38,46,46	3.27	9 (23%)	50,70,70	1.81	11 (22%)
31	CLA	g1	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	20 (26%)
31	CLA	s	614	-	55,63,73	1.47	7 (12%)	64,101,113	2.22	16 (25%)
31	CLA	R1	608	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	17 (24%)
31	CLA	R	603	-	60,68,73	1.43	10 (16%)	70,107,113	2.10	16 (22%)
31	CLA	Y1	610	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	15 (19%)
33	BCR	c1	514	-	41,41,41	1.83	4 (9%)	56,56,56	4.43	18 (32%)
31	CLA	b	613	-	65,73,73	1.35	6 (9%)	76,113,113	1.91	15 (19%)
56	ERG	r1	626	-	31,32,32	7.81	19 (61%)	47,50,50	3.08	18 (38%)
35	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.08	4 (6%)
31	CLA	C	501	-	65,73,73	1.35	9 (13%)	76,113,113	2.08	18 (23%)
47	CHL	s	608	-	61,69,74	0.85	3 (4%)	67,108,114	1.28	12 (17%)
31	CLA	R	610	-	60,68,73	1.39	7 (11%)	70,107,113	2.12	21 (30%)
31	CLA	y	608	-	50,58,73	1.56	8 (16%)	58,95,113	2.24	17 (29%)
47	CHL	S	601	-	46,54,74	1.04	3 (6%)	49,90,114	1.42	7 (14%)
41	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	0.98	2 (3%)
38	DGA	c	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.51	3 (6%)
31	CLA	n	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.09	19 (25%)
47	CHL	G	609	-	66,74,74	0.91	4 (6%)	73,114,114	1.21	11 (15%)
31	CLA	b1	613	-	65,73,73	1.39	8 (12%)	76,113,113	1.95	13 (17%)
49	XAT	g	622	-	39,47,47	0.68	1 (2%)	54,74,74	1.96	14 (25%)
47	CHL	y	606	-	66,74,74	0.87	3 (4%)	73,114,114	1.19	11 (15%)
31	CLA	C1	512	-	65,73,73	1.35	7 (10%)	76,113,113	2.09	19 (25%)
28	OEX	A1	401	1,4	0,15,15	-	-	-	-	-
31	CLA	y1	608	-	50,58,73	1.54	9 (18%)	58,95,113	2.26	17 (29%)
39	GOL	b	625	-	5,5,5	0.58	0	5,5,5	0.31	0
53	SPH	a1	414	-	19,20,20	0.66	0	18,21,21	1.03	1 (5%)
31	CLA	b1	609	-	65,73,73	1.37	8 (12%)	76,113,113	2.07	18 (23%)
38	DGA	B1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.44	3 (6%)
33	BCR	C	516	-	41,41,41	1.86	4 (9%)	56,56,56	4.36	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	LUT	Y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	1.98	11 (21%)
42	LMK	C	527	-	38,39,53	1.49	2 (5%)	41,46,60	1.27	2 (4%)
47	CHL	y1	606	-	66,74,74	0.85	3 (4%)	73,114,114	1.17	11 (15%)
35	LMG	A	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.14	3 (5%)
33	BCR	B	619	-	41,41,41	1.85	4 (9%)	56,56,56	4.34	20 (35%)
31	CLA	s	602	-	60,68,73	1.39	7 (11%)	70,107,113	2.04	15 (21%)
33	BCR	c1	517	-	41,41,41	1.81	4 (9%)	56,56,56	4.50	20 (35%)
32	PHO	a1	408	-	51,69,69	1.01	3 (5%)	47,99,99	1.15	4 (8%)
31	CLA	C	506	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	19 (25%)
31	CLA	R	602	-	60,68,73	1.41	7 (11%)	70,107,113	2.05	20 (28%)
31	CLA	B1	617	-	65,73,73	1.36	7 (10%)	76,113,113	1.93	17 (22%)
40	DGD	C1	519	-	63,63,67	1.13	7 (11%)	77,77,81	1.00	3 (3%)
47	CHL	s1	607	-	43,51,74	1.01	2 (4%)	45,86,114	1.46	7 (15%)
41	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
50	NEX	y1	623	-	38,46,46	3.30	9 (23%)	50,70,70	1.97	13 (26%)
34	SQD	m1	101	-	41,42,54	0.90	0	50,53,65	0.98	2 (4%)
31	CLA	c	503	-	65,73,73	1.37	8 (12%)	76,113,113	2.06	19 (25%)
31	CLA	S1	611	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
47	CHL	g	608	-	44,52,74	0.99	3 (6%)	46,87,114	1.51	10 (21%)
33	BCR	b	619	-	41,41,41	1.87	4 (9%)	56,56,56	4.43	19 (33%)
50	NEX	G	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.84	11 (22%)
31	CLA	B	602	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	16 (21%)
31	CLA	R1	609	-	60,68,73	1.39	8 (13%)	70,107,113	4.52	21 (30%)
47	CHL	g1	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.18	9 (12%)
35	LMG	w1	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.20	3 (6%)
48	LUT	g1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	11 (21%)
44	PL9	D1	405	-	55,55,55	0.99	5 (9%)	68,69,69	1.60	10 (14%)
31	CLA	c1	508	-	65,73,73	1.32	7 (10%)	76,113,113	1.97	14 (18%)
35	LMG	B1	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.12	3 (5%)
31	CLA	N	602	-	65,73,73	1.36	10 (15%)	76,113,113	1.98	19 (25%)
31	CLA	R	611	-	46,54,73	1.63	10 (21%)	53,90,113	2.18	14 (26%)
31	CLA	C	512	-	65,73,73	1.34	7 (10%)	76,113,113	1.90	17 (22%)
31	CLA	Y1	613	-	65,73,73	1.33	8 (12%)	76,113,113	2.10	18 (23%)
35	LMG	D	411	-	46,46,55	0.91	4 (8%)	54,54,63	1.17	4 (7%)
40	DGD	c1	519	-	63,63,67	1.12	7 (11%)	77,77,81	0.98	5 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMG	b	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.11	3 (5%)
32	PHO	a1	409	-	51,69,69	0.99	4 (7%)	47,99,99	1.28	6 (12%)
49	XAT	R1	621	-	39,47,47	0.64	1 (2%)	54,74,74	1.91	14 (25%)
31	CLA	R	613	-	46,54,73	1.61	9 (19%)	53,90,113	2.22	15 (28%)
31	CLA	y1	603	-	65,73,73	1.35	9 (13%)	76,113,113	2.03	17 (22%)
31	CLA	c	511	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	19 (25%)
47	CHL	S1	606	-	44,52,74	1.06	3 (6%)	46,87,114	1.38	8 (17%)
31	CLA	r1	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.06	16 (22%)
31	CLA	s1	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.03	13 (20%)
31	CLA	r	602	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	20 (28%)
35	LMG	D1	411	-	46,46,55	0.93	4 (8%)	54,54,63	1.07	2 (3%)
47	CHL	S	607	-	43,51,74	1.00	3 (6%)	45,86,114	1.46	9 (20%)
31	CLA	g1	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.27	15 (27%)
28	OEX	a	401	1,4	0,15,15	-	-	-	-	-
31	CLA	B1	610	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	19 (25%)
31	CLA	C1	509	-	65,73,73	1.31	6 (9%)	76,113,113	2.01	17 (22%)
41	LHG	l	101	-	48,48,48	0.39	0	51,54,54	0.96	2 (3%)
48	LUT	r1	620	-	42,43,43	2.37	1 (2%)	51,60,60	2.13	15 (29%)
47	CHL	s	607	-	43,51,74	0.99	2 (4%)	45,86,114	1.45	10 (22%)
33	BCR	c1	515	-	41,41,41	1.88	5 (12%)	56,56,56	4.30	16 (28%)
48	LUT	s	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.38	17 (33%)
31	CLA	B	604	-	65,73,73	1.38	9 (13%)	76,113,113	1.96	18 (23%)
31	CLA	C1	510	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	16 (21%)
34	SQD	a1	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)
31	CLA	n1	610	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	19 (25%)
31	CLA	G	604	-	49,57,73	1.58	9 (18%)	55,93,113	2.29	15 (27%)
31	CLA	r1	603	-	60,68,73	1.43	8 (13%)	70,107,113	2.00	15 (21%)
31	CLA	S1	604	-	55,63,73	1.47	7 (12%)	64,101,113	2.26	18 (28%)
39	GOL	I1	101	-	5,5,5	0.56	0	5,5,5	0.25	0
31	CLA	C1	513	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	20 (26%)
31	CLA	n1	603	-	65,73,73	1.36	10 (15%)	76,113,113	2.04	18 (23%)
31	CLA	g1	610	-	65,73,73	1.35	9 (13%)	76,113,113	1.98	19 (25%)
42	LMK	C1	527	-	38,39,53	1.51	2 (5%)	41,46,60	1.43	2 (4%)
46	RRX	H	101	-	42,42,42	11.48	26 (61%)	57,58,58	6.22	24 (42%)
31	CLA	Y	602	24	65,73,73	1.36	7 (10%)	76,113,113	1.92	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
43	BCT	D	401	29	2,3,3	1.16	0	2,3,3	4.53	2 (100%)
54	4RF	i1	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.91	3 (5%)
47	CHL	s1	606	-	44,52,74	0.95	2 (4%)	46,87,114	1.44	9 (19%)
31	CLA	R	609	-	60,68,73	1.43	8 (13%)	70,107,113	2.01	16 (22%)
32	PHO	a	408	-	51,69,69	1.02	4 (7%)	47,99,99	1.18	5 (10%)
49	XAT	n1	622	-	39,47,47	0.70	1 (2%)	54,74,74	1.88	14 (25%)
51	LPX	S1	625	-	29,29,29	1.03	2 (6%)	31,33,33	0.96	1 (3%)
31	CLA	B1	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.96	15 (19%)
31	CLA	C	502	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	16 (21%)
42	LMK	c1	527	-	38,39,53	1.49	2 (5%)	41,46,60	1.32	2 (4%)
31	CLA	Y	611	-	65,73,73	1.36	7 (10%)	76,113,113	1.90	14 (18%)
31	CLA	Y	603	-	65,73,73	1.33	9 (13%)	76,113,113	2.03	20 (26%)
48	LUT	n1	620	-	42,43,43	2.43	1 (2%)	51,60,60	1.80	13 (25%)
33	BCR	b	618	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	16 (28%)
33	BCR	B1	619	-	41,41,41	1.86	4 (9%)	56,56,56	4.42	15 (26%)
49	XAT	R	621	-	39,47,47	0.70	1 (2%)	54,74,74	2.03	14 (25%)
31	CLA	S	604	-	55,63,73	1.46	7 (12%)	64,101,113	2.16	17 (26%)
31	CLA	b1	606	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	19 (25%)
37	C7Z	B	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.21	17 (29%)
40	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.99	2 (2%)
47	CHL	n	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.30	12 (16%)
53	SPH	Y1	625	-	19,20,20	0.64	0	18,21,21	1.05	1 (5%)
49	XAT	Y1	622	-	39,47,47	0.69	1 (2%)	54,74,74	3.76	17 (31%)
41	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.07	2 (4%)
47	CHL	g1	605	-	48,56,74	0.96	2 (4%)	51,92,114	1.35	9 (17%)
31	CLA	c	509	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	15 (19%)
35	LMG	W1	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.21	2 (4%)
31	CLA	S	602	23	60,68,73	1.41	8 (13%)	70,107,113	2.02	15 (21%)
50	NEX	r	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.68	9 (18%)
31	CLA	C1	508	-	65,73,73	1.32	7 (10%)	76,113,113	1.99	18 (23%)
31	CLA	R1	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.33	13 (23%)
31	CLA	b	616	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	16 (21%)
47	CHL	R	607	-	50,58,74	0.94	2 (4%)	52,94,114	1.37	8 (15%)
49	XAT	N	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.90	13 (24%)
31	CLA	c	510	-	65,73,73	1.34	9 (13%)	76,113,113	2.04	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	3PH	t1	101	-	47,47,47	0.87	4 (8%)	51,52,52	1.11	2 (3%)
47	CHL	S	606	-	44,52,74	0.99	3 (6%)	46,87,114	1.43	9 (19%)
40	DGD	b1	623	-	44,44,67	0.87	2 (4%)	58,58,81	1.17	4 (6%)
31	CLA	n1	613	-	65,73,73	1.36	8 (12%)	76,113,113	2.09	18 (23%)
31	CLA	B	610	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	15 (19%)
31	CLA	c1	503	-	65,73,73	1.37	8 (12%)	76,113,113	2.06	20 (26%)
31	CLA	C	507	-	65,73,73	1.37	8 (12%)	76,113,113	1.94	18 (23%)
48	LUT	Y	620	-	42,43,43	2.38	1 (2%)	51,60,60	2.03	11 (21%)
48	LUT	N1	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.05	11 (21%)
31	CLA	y1	604	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
41	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
41	LHG	d1	408	-	43,43,48	0.41	0	46,49,54	1.06	3 (6%)
35	LMG	C1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.10	2 (3%)
33	BCR	C1	515	-	41,41,41	1.86	4 (9%)	56,56,56	4.37	14 (25%)
31	CLA	b1	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.18	18 (23%)
41	LHG	n1	624	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
31	CLA	S1	605	-	50,58,73	1.56	9 (18%)	58,95,113	2.29	18 (31%)
31	CLA	b1	610	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	14 (18%)
35	LMG	h1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.10	2 (3%)
31	CLA	b	612	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	18 (23%)
31	CLA	d1	402	-	65,73,73	1.37	9 (13%)	76,113,113	1.89	17 (22%)
31	CLA	N1	611	-	49,57,73	1.57	8 (16%)	55,93,113	2.20	14 (25%)
41	LHG	D	408	-	43,43,48	0.42	0	46,49,54	1.07	3 (6%)
31	CLA	Y1	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	16 (21%)
31	CLA	B1	613	-	65,73,73	1.34	8 (12%)	76,113,113	1.94	15 (19%)
47	CHL	n	601	-	66,74,74	0.82	3 (4%)	73,114,114	1.22	11 (15%)
37	C7Z	b1	620	-	43,43,43	5.33	26 (60%)	58,60,60	2.26	21 (36%)
34	SQD	c	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
49	XAT	y1	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.69	16 (29%)
31	CLA	g	612	-	43,51,73	1.68	9 (20%)	49,86,113	2.25	15 (30%)
31	CLA	g1	613	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	18 (23%)
35	LMG	a1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.05	2 (3%)
31	CLA	B	611	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
31	CLA	Y	604	-	65,73,73	1.35	9 (13%)	76,113,113	2.04	17 (22%)
48	LUT	R	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.14	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	A	407	-	49,57,73	1.56	9 (18%)	55,93,113	2.22	15 (27%)
31	CLA	B	613	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	15 (19%)
31	CLA	s	605	-	50,58,73	1.57	9 (18%)	58,95,113	2.33	19 (32%)
34	SQD	b1	621	-	41,42,54	0.88	0	50,53,65	0.96	2 (4%)
31	CLA	b1	612	-	65,73,73	1.34	6 (9%)	76,113,113	2.04	17 (22%)
47	CHL	n1	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.28	11 (15%)
50	NEX	r1	622	-	38,46,46	3.39	10 (26%)	50,70,70	1.74	11 (22%)
45	HEM	F	101	7,6	41,50,50	1.51	3 (7%)	45,82,82	1.55	8 (17%)
47	CHL	g1	608	-	44,52,74	1.02	3 (6%)	46,87,114	1.37	9 (19%)
47	CHL	n1	601	20	66,74,74	0.81	3 (4%)	73,114,114	1.21	8 (10%)
52	3PH	s	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
47	CHL	G1	608	-	44,52,74	1.01	3 (6%)	46,87,114	1.49	9 (19%)
31	CLA	r	612	-	60,68,73	1.43	9 (15%)	70,107,113	1.98	15 (21%)
31	CLA	a	406	-	65,73,73	1.32	6 (9%)	76,113,113	2.05	16 (21%)
33	BCR	B	618	-	41,41,41	1.82	4 (9%)	56,56,56	4.40	14 (25%)
47	CHL	Y	609	-	66,74,74	0.83	3 (4%)	73,114,114	1.22	12 (16%)
47	CHL	s1	608	-	61,69,74	0.87	3 (4%)	67,108,114	1.27	10 (14%)
38	DGA	C	524	-	43,43,43	1.12	3 (6%)	45,45,45	1.51	3 (6%)
45	HEM	f	101	7,6	41,50,50	1.53	3 (7%)	45,82,82	1.54	9 (20%)
31	CLA	N	611	-	49,57,73	1.58	10 (20%)	55,93,113	2.30	16 (29%)
31	CLA	n	603	-	65,73,73	1.35	7 (10%)	76,113,113	2.11	17 (22%)
31	CLA	g	611	-	45,53,73	1.62	8 (17%)	52,89,113	2.26	15 (28%)
31	CLA	g	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	16 (21%)
31	CLA	b1	611	-	65,73,73	1.34	8 (12%)	76,113,113	1.93	16 (21%)
47	CHL	y1	607	-	66,74,74	0.76	2 (3%)	73,114,114	1.25	10 (13%)
31	CLA	r	611	-	46,54,73	1.62	10 (21%)	53,90,113	2.14	14 (26%)
49	XAT	G1	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.88	14 (25%)
50	NEX	Y1	623	-	38,46,46	3.37	10 (26%)	50,70,70	2.02	12 (24%)
31	CLA	b	615	-	65,73,73	1.36	8 (12%)	76,113,113	2.19	21 (27%)
31	CLA	s	617	-	50,58,73	1.53	9 (18%)	58,95,113	2.26	18 (31%)
50	NEX	n	623	-	38,46,46	3.38	9 (23%)	50,70,70	1.77	13 (26%)
48	LUT	g	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.09	12 (23%)
47	CHL	r1	606	-	44,52,74	1.04	2 (4%)	46,87,114	1.25	5 (10%)
33	BCR	C1	516	-	41,41,41	1.67	5 (12%)	56,56,56	4.31	17 (30%)
31	CLA	g	610	-	65,73,73	1.33	6 (9%)	76,113,113	2.03	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LMG	j	101	-	45,45,55	0.91	3 (6%)	53,53,63	1.05	2 (3%)
40	DGD	c	520	-	60,60,67	1.06	5 (8%)	74,74,81	1.02	2 (2%)
31	CLA	r	613	-	46,54,73	1.60	8 (17%)	53,90,113	2.22	14 (26%)
31	CLA	a	405	-	65,73,73	1.33	6 (9%)	76,113,113	2.06	19 (25%)
31	CLA	y	611	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
31	CLA	c1	504	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	17 (22%)
31	CLA	D	402	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	15 (19%)
31	CLA	b	607	-	65,73,73	1.38	8 (12%)	76,113,113	2.09	17 (22%)
49	XAT	G	622	-	39,47,47	0.71	1 (2%)	54,74,74	1.88	13 (24%)
47	CHL	N1	608	-	50,58,74	0.94	3 (6%)	52,94,114	1.48	11 (21%)
40	DGD	c1	520	-	60,60,67	1.08	4 (6%)	74,74,81	1.00	3 (4%)
48	LUT	S1	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.02	10 (19%)
31	CLA	y	610	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	19 (25%)
31	CLA	R	604	-	49,57,73	1.55	7 (14%)	55,93,113	2.27	18 (32%)
48	LUT	Y	621	-	42,43,43	2.30	1 (2%)	51,60,60	1.98	15 (29%)
31	CLA	r1	612	-	60,68,73	1.44	10 (16%)	70,107,113	2.02	17 (24%)
31	CLA	g1	604	-	49,57,73	1.57	8 (16%)	55,93,113	2.22	19 (34%)
31	CLA	R1	603	-	60,68,73	1.44	9 (15%)	70,107,113	1.95	15 (21%)
47	CHL	y1	605	-	46,54,74	0.97	3 (6%)	49,90,114	1.42	7 (14%)
31	CLA	s	613	-	55,63,73	1.48	7 (12%)	64,101,113	2.28	14 (21%)
48	LUT	G	621	-	42,43,43	2.38	1 (2%)	51,60,60	2.07	16 (31%)
31	CLA	n1	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.28	18 (32%)
47	CHL	S	608	-	61,69,74	0.86	3 (4%)	67,108,114	1.26	10 (14%)
31	CLA	b1	615	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	16 (21%)
34	SQD	M1	101	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
31	CLA	B	609	-	65,73,73	1.38	8 (12%)	76,113,113	2.09	21 (27%)
41	LHG	L1	101	-	48,48,48	0.38	0	51,54,54	4.47	5 (9%)
31	CLA	y1	610	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
50	NEX	N1	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.72	13 (26%)
48	LUT	n	620	-	42,43,43	2.36	1 (2%)	51,60,60	2.11	13 (25%)
31	CLA	n	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.07	21 (27%)
31	CLA	N1	612	-	45,53,73	1.62	8 (17%)	52,89,113	2.15	13 (25%)
31	CLA	Y1	611	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	14 (18%)
31	CLA	Y1	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	18 (23%)
31	CLA	a1	410	-	60,68,73	1.39	7 (11%)	70,107,113	2.06	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	3PH	s1	626	-	47,47,47	0.88	4 (8%)	51,52,52	4.43	4 (7%)
31	CLA	C	509	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
48	LUT	n	621	-	42,43,43	2.39	1 (2%)	51,60,60	2.00	12 (23%)
40	DGD	C	523	-	67,67,67	1.18	7 (10%)	81,81,81	1.07	3 (3%)
31	CLA	N	614	-	49,57,73	1.55	9 (18%)	55,93,113	2.25	16 (29%)
31	CLA	c	506	-	65,73,73	1.38	8 (12%)	76,113,113	2.03	19 (25%)
47	CHL	n1	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.17	9 (12%)
47	CHL	R	606	-	44,52,74	1.04	3 (6%)	46,87,114	1.32	8 (17%)
31	CLA	C	510	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	15 (19%)
31	CLA	r	609	-	60,68,73	1.41	7 (11%)	70,107,113	2.03	17 (24%)
47	CHL	N	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.38	9 (17%)
31	CLA	b1	614	-	65,73,73	1.35	8 (12%)	76,113,113	1.92	18 (23%)
48	LUT	y	621	-	42,43,43	2.30	1 (2%)	51,60,60	2.02	12 (23%)
31	CLA	s1	605	23	50,58,73	1.58	8 (16%)	58,95,113	2.28	17 (29%)
31	CLA	S1	610	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	20 (26%)
46	RRX	h1	101	-	42,42,42	4.93	24 (57%)	57,58,58	2.53	21 (36%)
31	CLA	C	513	-	65,73,73	1.33	7 (10%)	76,113,113	2.07	18 (23%)
31	CLA	y	604	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	17 (22%)
47	CHL	N	605	-	66,74,74	0.86	3 (4%)	73,114,114	1.16	9 (12%)
31	CLA	C	511	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	19 (25%)
31	CLA	s1	617	-	50,58,73	1.52	8 (16%)	58,95,113	2.27	19 (32%)
47	CHL	G	605	21	48,56,74	0.94	2 (4%)	51,92,114	1.39	11 (21%)
31	CLA	s	604	-	55,63,73	1.47	8 (14%)	64,101,113	2.17	18 (28%)
31	CLA	g	614	-	49,57,73	1.56	8 (16%)	55,93,113	2.28	17 (30%)
50	NEX	g	623	-	38,46,46	3.32	10 (26%)	50,70,70	1.84	14 (28%)
31	CLA	B	607	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	18 (23%)
31	CLA	y	613	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	17 (22%)
31	CLA	y	614	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
48	LUT	Y1	620	-	42,43,43	2.37	1 (2%)	51,60,60	2.01	14 (27%)
32	PHO	A1	408	-	51,69,69	0.99	4 (7%)	47,99,99	1.12	5 (10%)
31	CLA	y1	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	16 (21%)
33	BCR	B1	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.50	18 (32%)
31	CLA	y1	613	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	17 (22%)
48	LUT	N	620	-	42,43,43	2.37	1 (2%)	51,60,60	2.07	15 (29%)
31	CLA	Y	614	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	b	606	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	14 (18%)
31	CLA	C1	502	-	65,73,73	1.39	8 (12%)	76,113,113	1.94	15 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	h	102	-	-	13/43/63/70	0/1/1/1
31	CLA	b	614	-	1/1/15/20	17/37/115/115	-
47	CHL	n1	605	-	4/4/20/26	11/39/137/137	-
31	CLA	C1	504	-	1/1/15/20	15/37/115/115	-
31	CLA	b1	607	-	1/1/15/20	16/37/115/115	-
41	LHG	C1	525	-	-	32/51/51/53	-
45	HEM	F1	101	6	-	1/12/54/54	-
47	CHL	Y	605	24	3/3/16/26	1/15/113/137	-
48	LUT	S1	621	-	-	3/29/67/67	0/2/2/2
31	CLA	N	604	-	1/1/15/20	17/37/115/115	-
48	LUT	G1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	c1	502	-	1/1/15/20	14/37/115/115	-
34	SQD	b1	626	-	-	23/49/69/69	0/1/1/1
49	XAT	y	622	-	-	3/31/93/93	0/4/4/4
57	PTY	y1	627	-	-	14/20/20/53	-
31	CLA	c	508	-	1/1/15/20	13/37/115/115	-
32	PHO	a	409	-	-	11/37/103/103	0/5/6/6
41	LHG	D1	408	-	-	30/48/48/53	-
41	LHG	Y	624	-	-	32/53/53/53	-
31	CLA	n	614	-	1/1/11/20	5/18/96/115	-
31	CLA	n1	602	-	1/1/15/20	18/37/115/115	-
38	DGA	J1	101	-	-	11/30/30/45	-
31	CLA	B1	603	-	1/1/15/20	18/37/115/115	-
31	CLA	S	617	-	1/1/12/20	9/19/97/115	-
35	LMG	d1	411	-	-	12/41/61/70	0/1/1/1
31	CLA	n1	604	-	1/1/15/20	14/37/115/115	-
31	CLA	r1	602	-	1/1/14/20	13/31/109/115	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	LUT	s1	621	-	-	2/29/67/67	0/2/2/2
31	CLA	Y	612	-	1/1/15/20	9/37/115/115	-
31	CLA	d1	403	-	1/1/15/20	11/37/115/115	-
31	CLA	B1	609	-	1/1/15/20	15/37/115/115	-
31	CLA	A1	406	-	1/1/15/20	16/37/115/115	-
31	CLA	c1	505	-	1/1/15/20	17/37/115/115	-
31	CLA	s1	610	-	1/1/15/20	17/37/115/115	-
49	XAT	g1	622	-	2/2/12/26	0/31/93/93	0/4/4/4
33	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
47	CHL	Y	601	-	4/4/20/26	7/39/137/137	-
35	LMG	c1	523	-	-	14/50/70/70	0/1/1/1
47	CHL	n	605	-	4/4/20/26	5/39/137/137	-
47	CHL	g	601	21	4/4/20/26	7/39/137/137	-
40	DGD	c	519	-	-	22/51/91/95	0/2/2/2
34	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
52	3PH	S1	626	-	-	23/49/49/49	-
31	CLA	r1	608	-	1/1/14/20	22/31/109/115	-
33	BCR	C1	517	-	-	12/29/63/63	0/2/2/2
31	CLA	c1	507	-	1/1/15/20	19/37/115/115	-
47	CHL	n1	606	-	4/4/20/26	5/39/137/137	-
31	CLA	a	407	-	1/1/11/20	5/18/96/115	-
31	CLA	c	502	-	1/1/15/20	13/37/115/115	-
31	CLA	C1	506	-	1/1/15/20	19/37/115/115	-
33	BCR	c	515	-	-	11/29/63/63	0/2/2/2
47	CHL	y1	609	-	4/4/20/26	9/39/137/137	-
35	LMG	c	521	-	-	20/46/66/70	0/1/1/1
31	CLA	A	406	-	1/1/15/20	16/37/115/115	-
47	CHL	Y	606	-	4/4/20/26	6/39/137/137	-
31	CLA	G	611	-	1/1/11/20	4/13/91/115	-
31	CLA	N1	610	-	1/1/15/20	18/37/115/115	-
47	CHL	Y1	601	24	4/4/20/26	2/39/137/137	-
33	BCR	c	517	-	-	11/29/63/63	0/2/2/2
33	BCR	C	517	-	-	8/29/63/63	0/2/2/2
34	SQD	c1	526	-	-	17/49/69/69	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	d	404	-	-	11/29/63/63	0/2/2/2
31	CLA	a1	405	-	1/1/15/20	14/37/115/115	-
31	CLA	R	612	-	1/1/14/20	13/31/109/115	-
48	LUT	S	621	-	-	1/29/67/67	0/2/2/2
35	LMG	c1	521	-	-	12/46/66/70	0/1/1/1
31	CLA	S	610	-	1/1/15/20	14/37/115/115	-
47	CHL	Y1	607	-	4/4/20/26	8/39/137/137	-
31	CLA	R1	602	-	1/1/14/20	13/31/109/115	-
31	CLA	Y	608	-	1/1/12/20	6/19/97/115	-
47	CHL	N	601	20	4/4/20/26	5/39/137/137	-
50	NEX	Y	623	-	-	3/27/83/83	0/3/3/3
41	LHG	D1	409	-	-	31/53/53/53	-
35	LMG	A1	413	-	-	14/43/63/70	0/1/1/1
31	CLA	b1	605	-	1/1/15/20	19/37/115/115	-
47	CHL	G	606	-	4/4/16/26	6/20/118/137	-
37	C7Z	b	620	-	1/1/12/26	8/29/67/67	0/2/2/2
31	CLA	c1	510	-	1/1/15/20	17/37/115/115	-
47	CHL	R1	607	-	3/3/16/26	6/20/118/137	-
31	CLA	s1	611	-	1/1/15/20	15/37/115/115	-
47	CHL	r1	607	-	3/3/16/26	6/20/118/137	-
31	CLA	S1	614	-	1/1/13/20	10/25/103/115	-
31	CLA	G1	610	-	1/1/15/20	14/37/115/115	-
31	CLA	C1	503	-	1/1/15/20	15/37/115/115	-
31	CLA	c1	506	-	1/1/15/20	17/37/115/115	-
38	DGA	b	623	-	-	27/45/45/45	-
54	4RF	k1	101	-	-	35/59/59/59	-
38	DGA	B	625	-	-	28/45/45/45	-
31	CLA	g1	611	-	1/1/15/20	16/37/115/115	-
31	CLA	g1	603	-	1/1/15/20	20/37/115/115	-
31	CLA	b	602	-	1/1/15/20	23/37/115/115	-
47	CHL	g	605	-	3/3/16/26	3/18/116/137	-
31	CLA	S1	613	-	1/1/13/20	8/25/103/115	-
31	CLA	Y1	608	-	1/1/12/20	9/19/97/115	-
47	CHL	Y1	609	-	4/4/20/26	9/39/137/137	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SQD	a	412	-	-	13/46/66/69	0/1/1/1
31	CLA	y1	602	-	1/1/15/20	16/37/115/115	-
48	LUT	N1	620	-	-	5/29/67/67	0/2/2/2
56	ERG	R1	626	-	5/5/11/15	7/13/71/71	0/4/4/4
31	CLA	b	608	-	1/1/15/20	25/37/115/115	-
31	CLA	d	403	-	1/1/15/20	11/37/115/115	-
47	CHL	y	605	24	3/3/16/26	6/15/113/137	-
57	PTY	Y1	627	-	-	12/20/20/53	-
40	DGD	C	518	-	-	12/44/84/95	0/2/2/2
41	LHG	S1	624	-	-	27/49/49/53	-
50	NEX	R	622	-	-	11/27/83/83	0/3/3/3
31	CLA	B1	615	-	1/1/15/20	17/37/115/115	-
55	LMT	R1	625	-	-	9/21/61/61	0/2/2/2
50	NEX	N	623	-	-	7/27/83/83	0/3/3/3
47	CHL	n	607	-	4/4/20/26	11/39/137/137	-
31	CLA	A1	410	-	1/1/14/20	8/31/109/115	-
31	CLA	N1	613	-	1/1/15/20	18/37/115/115	-
47	CHL	N1	607	-	4/4/20/26	6/39/137/137	-
47	CHL	G1	605	-	4/4/16/26	5/18/116/137	-
31	CLA	S	611	-	1/1/15/20	16/37/115/115	-
31	CLA	S1	602	-	1/1/14/20	17/31/109/115	-
31	CLA	c1	512	-	1/1/15/20	17/37/115/115	-
31	CLA	S1	612	-	1/1/11/20	6/13/91/115	-
47	CHL	G	608	-	3/3/15/26	0/13/111/137	-
47	CHL	S1	601	23	3/3/16/26	2/15/113/137	-
31	CLA	N	603	-	1/1/15/20	13/37/115/115	-
41	LHG	n	624	-	-	31/53/53/53	-
33	BCR	a	411	-	-	10/29/63/63	0/2/2/2
48	LUT	y	620	-	-	2/29/67/67	0/2/2/2
31	CLA	A1	405	-	1/1/15/20	14/37/115/115	-
33	BCR	C1	514	-	-	16/29/63/63	0/2/2/2
48	LUT	G1	621	-	-	4/29/67/67	0/2/2/2
40	DGD	C	519	-	-	18/51/91/95	0/2/2/2
41	LHG	d1	410	-	-	25/43/43/53	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	NEX	R1	622	-	-	6/27/83/83	0/3/3/3
47	CHL	r	606	-	3/3/15/26	1/13/111/137	-
31	CLA	S	614	-	1/1/13/20	8/25/103/115	-
31	CLA	B	612	-	1/1/15/20	22/37/115/115	-
49	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
33	BCR	A1	411	-	-	12/29/63/63	0/2/2/2
31	CLA	Y1	614	-	1/1/15/20	14/37/115/115	-
57	PTY	y1	626	-	-	24/53/53/53	-
31	CLA	s	611	-	1/1/15/20	16/37/115/115	-
31	CLA	s	603	-	1/1/15/20	18/37/115/115	-
53	SPH	Y	625	-	-	12/21/21/21	-
31	CLA	s1	613	-	1/1/13/20	9/25/103/115	-
31	CLA	n	610	-	1/1/15/20	16/37/115/115	-
32	PHO	A	408	-	-	6/37/103/103	0/5/6/6
31	CLA	B1	605	-	1/1/15/20	14/37/115/115	-
31	CLA	C	503	-	1/1/15/20	20/37/115/115	-
47	CHL	S1	608	-	4/4/19/26	10/33/131/137	-
41	LHG	y1	624	-	-	27/53/53/53	-
31	CLA	n	611	-	1/1/11/20	13/18/96/115	-
35	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
35	LMG	B	622	-	-	11/39/59/70	0/1/1/1
31	CLA	N	610	-	1/1/15/20	9/37/115/115	-
33	BCR	C	515	-	-	11/29/63/63	0/2/2/2
47	CHL	Y1	606	-	4/4/20/26	8/39/137/137	-
31	CLA	g	613	-	1/1/15/20	18/37/115/115	-
33	BCR	D	404	-	-	13/29/63/63	0/2/2/2
37	C7Z	B1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
31	CLA	G	613	-	1/1/15/20	18/37/115/115	-
31	CLA	c	512	-	1/1/15/20	21/37/115/115	-
50	NEX	S1	623	-	-	3/27/83/83	0/3/3/3
48	LUT	g	620	-	-	6/29/67/67	0/2/2/2
41	LHG	Y1	624	-	-	26/53/53/53	-
31	CLA	r	603	-	1/1/14/20	14/31/109/115	-
31	CLA	R1	612	-	1/1/14/20	14/31/109/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	G	601	-	4/4/20/26	6/39/137/137	-
47	CHL	n	606	-	4/4/20/26	5/39/137/137	-
47	CHL	g	606	-	3/3/16/26	6/20/118/137	-
48	LUT	g1	621	-	1/1/12/27	3/29/67/67	0/2/2/2
47	CHL	S1	607	-	3/3/15/26	3/12/110/137	-
31	CLA	B1	612	-	1/1/15/20	11/37/115/115	-
31	CLA	y	612	-	1/1/15/20	12/37/115/115	-
31	CLA	C	508	-	1/1/15/20	15/37/115/115	-
31	CLA	S	613	-	1/1/13/20	9/25/103/115	-
31	CLA	y1	614	-	1/1/15/20	11/37/115/115	-
31	CLA	G1	613	-	1/1/15/20	11/37/115/115	-
31	CLA	s	609	-	1/1/14/20	14/31/109/115	-
31	CLA	B	615	-	1/1/15/20	10/37/115/115	-
53	SPH	y1	625	-	-	11/21/21/21	-
31	CLA	B	617	-	1/1/15/20	16/37/115/115	-
31	CLA	s1	604	-	1/1/13/20	12/25/103/115	-
31	CLA	c	513	-	1/1/15/20	21/37/115/115	-
47	CHL	N1	601	20	4/4/20/26	3/39/137/137	-
51	LPX	S	625	-	-	13/31/31/31	-
41	LHG	d	410	-	-	32/43/43/53	-
39	GOL	B	627	-	-	0/4/4/4	-
31	CLA	Y1	604	-	1/1/15/20	18/37/115/115	-
31	CLA	n	604	-	1/1/15/20	15/37/115/115	-
41	LHG	N1	624	-	-	39/53/53/53	-
31	CLA	G1	614	-	1/1/11/20	11/18/96/115	-
47	CHL	R1	606	-	3/3/15/26	2/13/111/137	-
41	LHG	c1	525	-	-	35/51/51/53	-
50	NEX	G1	623	-	-	2/27/83/83	0/3/3/3
33	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
47	CHL	Y	607	-	4/4/20/26	8/39/137/137	-
34	SQD	A	412	-	-	18/46/66/69	0/1/1/1
35	LMG	J	101	-	-	15/40/60/70	0/1/1/1
31	CLA	c	507	-	1/1/15/20	20/37/115/115	-
35	LMG	d	411	-	-	9/41/61/70	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SQD	C1	526	-	-	24/49/69/69	0/1/1/1
54	4RF	I1	102	-	-	35/59/59/59	-
52	3PH	i	101	-	-	21/49/49/49	-
31	CLA	g	604	-	1/1/11/20	8/18/96/115	-
47	CHL	G1	601	21	4/4/20/26	11/39/137/137	-
31	CLA	N	613	-	1/1/15/20	18/37/115/115	-
47	CHL	Y1	605	24	3/3/16/26	1/15/113/137	-
52	3PH	T1	101	-	-	29/49/49/49	-
34	SQD	B1	626	-	-	24/49/69/69	0/1/1/1
41	LHG	L	101	-	-	33/53/53/53	-
31	CLA	R	608	-	1/1/14/20	17/31/109/115	-
31	CLA	A	410	-	1/1/14/20	10/31/109/115	-
47	CHL	G1	607	-	4/4/20/26	12/39/137/137	-
31	CLA	G	612	-	1/1/10/20	4/11/89/115	-
52	3PH	B1	624	-	-	23/49/49/49	-
31	CLA	s	610	-	1/1/15/20	22/37/115/115	-
48	LUT	S	620	-	1/1/12/27	3/29/67/67	0/2/2/2
55	LMT	r1	625	-	-	9/21/61/61	0/2/2/2
31	CLA	d	402	-	1/1/15/20	17/37/115/115	-
42	LMK	c	627	-	1/1/6/6	11/46/46/60	-
31	CLA	Y1	602	-	1/1/15/20	20/37/115/115	-
47	CHL	N1	609	-	4/4/20/26	8/39/137/137	-
31	CLA	G1	604	-	1/1/11/20	8/18/96/115	-
31	CLA	y	603	-	1/1/15/20	10/37/115/115	-
31	CLA	G1	612	-	1/1/10/20	5/11/89/115	-
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
31	CLA	B	616	-	1/1/15/20	13/37/115/115	-
48	LUT	R1	620	-	1/1/12/27	5/29/67/67	0/2/2/2
49	XAT	Y	622	-	1/1/12/26	4/31/93/93	0/4/4/4
47	CHL	g1	609	-	4/4/20/26	5/39/137/137	-
31	CLA	y1	612	-	1/1/15/20	13/37/115/115	-
31	CLA	C1	507	-	1/1/15/20	16/37/115/115	-
31	CLA	B1	606	-	1/1/15/20	7/37/115/115	-
49	XAT	n	622	-	-	2/31/93/93	0/4/4/4

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	H1	102	-	-	14/43/63/70	0/1/1/1
32	PHO	A1	409	-	-	14/37/103/103	0/5/6/6
31	CLA	b1	602	-	1/1/15/20	18/37/115/115	-
47	CHL	y	609	-	4/4/20/26	6/39/137/137	-
41	LHG	s1	624	-	-	24/49/49/53	-
31	CLA	S1	609	-	1/1/14/20	12/31/109/115	-
41	LHG	d1	409	-	-	32/53/53/53	-
31	CLA	r	604	-	1/1/11/20	9/18/96/115	-
48	LUT	s	621	-	-	1/29/67/67	0/2/2/2
31	CLA	g	602	-	1/1/15/20	22/37/115/115	-
31	CLA	C1	505	-	1/1/15/20	19/37/115/115	-
41	LHG	g1	624	-	-	30/53/53/53	-
57	PTY	Y1	626	-	-	19/53/53/53	-
31	CLA	a1	406	-	1/1/15/20	16/37/115/115	-
47	CHL	N	609	-	4/4/20/26	8/39/137/137	-
31	CLA	b1	604	-	1/1/15/20	16/37/115/115	-
31	CLA	N1	614	-	1/1/11/20	5/18/96/115	-
48	LUT	n1	621	-	-	3/29/67/67	0/2/2/2
31	CLA	n	612	-	1/1/11/20	3/13/91/115	-
39	GOL	y	626	-	-	0/4/4/4	-
40	DGD	C1	520	-	-	14/48/88/95	0/2/2/2
31	CLA	r	608	-	1/1/14/20	15/31/109/115	-
47	CHL	n	608	-	3/3/16/26	5/20/118/137	-
31	CLA	c1	509	-	1/1/15/20	15/37/115/115	-
33	BCR	D1	404	-	-	11/29/63/63	0/2/2/2
31	CLA	b	605	-	1/1/15/20	18/37/115/115	-
38	DGA	j1	101	-	-	15/30/30/45	-
31	CLA	A1	407	-	1/1/12/20	9/19/97/115	-
33	BCR	b1	618	-	-	8/29/63/63	0/2/2/2
31	CLA	r1	610	-	1/1/14/20	17/31/109/115	-
38	DGA	c1	524	-	-	23/45/45/45	-
45	HEM	f1	101	-	-	0/12/54/54	-
44	PL9	d	405	-	-	10/53/73/73	0/1/1/1
31	CLA	G1	611	-	1/1/15/20	15/37/115/115	-
31	CLA	b1	616	-	1/1/15/20	9/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	617	-	1/1/15/20	14/37/115/115	-
38	DGA	C1	524	-	-	34/45/45/45	-
41	LHG	g	624	-	-	28/53/53/53	-
44	PL9	D	405	-	-	20/53/73/73	0/1/1/1
31	CLA	n1	611	-	1/1/11/20	11/18/96/115	-
41	LHG	D	410	-	-	27/43/43/53	-
31	CLA	s1	603	-	1/1/15/20	17/37/115/115	-
48	LUT	N	621	-	-	3/29/67/67	0/2/2/2
49	XAT	r	622	-	1/1/12/26	12/31/93/93	0/4/4/4
31	CLA	c1	513	-	1/1/15/20	20/37/115/115	-
31	CLA	G	603	-	1/1/15/20	22/37/115/115	-
31	CLA	c1	511	-	1/1/15/20	13/37/115/115	-
31	CLA	S1	603	-	1/1/15/20	17/37/115/115	-
50	NEX	y	623	-	-	5/27/83/83	0/3/3/3
31	CLA	N1	602	-	1/1/15/20	12/37/115/115	-
41	LHG	y	624	-	-	28/53/53/53	-
31	CLA	C1	501	-	1/1/15/20	12/37/115/115	-
31	CLA	G	610	-	1/1/15/20	13/37/115/115	-
40	DGD	B1	623	-	-	16/32/72/95	0/2/2/2
31	CLA	Y	610	-	1/1/15/20	18/37/115/115	-
31	CLA	C	504	-	1/1/15/20	15/37/115/115	-
50	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	c1	501	-	1/1/15/20	18/37/115/115	-
47	CHL	s1	601	23	3/3/16/26	3/15/113/137	-
31	CLA	B1	604	-	1/1/15/20	19/37/115/115	-
52	3PH	b1	624	-	-	21/49/49/49	-
31	CLA	B	614	-	1/1/15/20	13/37/115/115	-
47	CHL	N	607	-	4/4/20/26	8/39/137/137	-
47	CHL	g	607	-	3/3/16/26	3/20/118/137	-
47	CHL	y	601	24	4/4/20/26	9/39/137/137	-
31	CLA	B	605	-	1/1/15/20	18/37/115/115	-
31	CLA	c	505	-	1/1/15/20	19/37/115/115	-
39	GOL	b	624	-	-	1/4/4/4	-
31	CLA	D	403	-	1/1/15/20	15/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	c	516	-	-	12/29/63/63	0/2/2/2
47	CHL	g1	601	-	4/4/20/26	17/39/137/137	-
31	CLA	s1	612	-	1/1/11/20	6/13/91/115	-
31	CLA	B	606	-	1/1/15/20	14/37/115/115	-
50	NEX	g1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	N1	603	-	1/1/15/20	16/37/115/115	-
31	CLA	G1	602	-	1/1/15/20	19/37/115/115	-
41	LHG	N	624	-	-	27/53/53/53	-
31	CLA	c	504	-	1/1/15/20	13/37/115/115	-
34	SQD	B1	621	-	-	14/37/57/69	0/1/1/1
47	CHL	y	607	-	4/4/20/26	7/39/137/137	-
41	LHG	d	408	-	-	30/48/48/53	-
31	CLA	g1	612	-	1/1/10/20	4/11/89/115	-
47	CHL	N1	606	-	4/4/20/26	12/39/137/137	-
31	CLA	S	603	-	1/1/15/20	10/37/115/115	-
34	SQD	b	621	-	-	19/49/69/69	0/1/1/1
35	LMG	a	413	-	-	18/43/63/70	0/1/1/1
48	LUT	G	620	-	-	3/29/67/67	0/2/2/2
31	CLA	G	602	-	1/1/15/20	22/37/115/115	-
31	CLA	A	405	-	1/1/15/20	12/37/115/115	-
31	CLA	S	609	-	1/1/14/20	12/31/109/115	-
47	CHL	N1	605	20	4/4/20/26	5/39/137/137	-
31	CLA	b	610	-	1/1/15/20	16/37/115/115	-
35	LMG	H	102	-	-	10/43/63/70	0/1/1/1
48	LUT	y1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	B1	608	-	1/1/15/20	24/37/115/115	-
31	CLA	C1	511	-	1/1/15/20	12/37/115/115	-
31	CLA	b	611	-	1/1/15/20	10/37/115/115	-
47	CHL	s	606	-	3/3/15/26	1/13/111/137	-
48	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
41	LHG	c	625	-	-	34/51/51/53	-
31	CLA	c	501	-	1/1/15/20	17/37/115/115	-
47	CHL	g1	606	-	3/3/16/26	4/20/118/137	-
40	DGD	C1	518	-	-	14/44/84/95	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	n1	608	-	3/3/16/26	3/20/118/137	-
41	LHG	s	624	-	-	27/49/49/53	-
47	CHL	G1	606	-	3/3/16/26	2/20/118/137	-
38	DGA	b1	625	-	-	23/45/45/45	-
49	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
31	CLA	B	608	-	1/1/15/20	21/37/115/115	-
31	CLA	r	610	-	1/1/14/20	15/31/109/115	-
51	LPX	s1	625	-	-	15/31/31/31	-
31	CLA	Y	613	-	1/1/15/20	21/37/115/115	-
46	RRX	H1	101	-	1/1/11/25	5/29/65/65	0/2/2/2
31	CLA	s	612	-	1/1/11/20	8/13/91/115	-
31	CLA	a1	407	-	1/1/11/20	7/18/96/115	-
31	CLA	N1	604	-	1/1/15/20	13/37/115/115	-
40	DGD	c	518	-	-	8/44/84/95	0/2/2/2
47	CHL	s	601	23	3/3/16/26	5/15/113/137	-
50	NEX	n1	623	-	-	4/27/83/83	1/3/3/3
31	CLA	S	612	-	1/1/11/20	4/13/91/115	-
31	CLA	b1	617	-	1/1/15/20	17/37/115/115	-
40	DGD	c	523	-	-	16/55/95/95	0/2/2/2
54	4RF	K1	101	-	-	31/59/59/59	-
40	DGD	c1	518	-	-	16/44/84/95	0/2/2/2
46	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2
35	LMG	b1	622	-	-	15/39/59/70	0/1/1/1
31	CLA	r1	604	-	1/1/11/20	9/18/96/115	-
31	CLA	B1	611	-	1/1/15/20	14/37/115/115	-
47	CHL	N	606	-	4/4/20/26	5/39/137/137	-
47	CHL	G	607	-	3/3/16/26	3/20/118/137	-
53	SPH	A1	414	-	-	13/21/21/21	-
52	3PH	S	626	-	-	19/49/49/49	-
31	CLA	G1	603	-	1/1/15/20	17/37/115/115	-
31	CLA	b	603	-	1/1/15/20	19/37/115/115	-
31	CLA	R1	610	-	1/1/14/20	13/31/109/115	-
31	CLA	s1	609	-	1/1/14/20	14/31/109/115	-
31	CLA	D1	402	-	1/1/15/20	22/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	a	410	-	1/1/14/20	9/31/109/115	-
31	CLA	N	612	-	1/1/11/20	6/13/91/115	-
31	CLA	B1	616	-	1/1/15/20	12/37/115/115	-
33	BCR	b1	619	-	-	7/29/63/63	0/2/2/2
48	LUT	r	620	-	-	8/29/67/67	0/2/2/2
31	CLA	B	603	-	1/1/15/20	19/37/115/115	-
31	CLA	B1	614	-	1/1/15/20	11/37/115/115	-
31	CLA	b	609	-	1/1/15/20	11/37/115/115	-
47	CHL	r	607	-	3/3/16/26	6/20/118/137	-
41	LHG	D1	410	-	-	22/43/43/53	-
31	CLA	D1	403	-	1/1/15/20	17/37/115/115	-
47	CHL	G1	609	-	4/4/20/26	9/39/137/137	-
34	SQD	C	526	-	-	17/49/69/69	0/1/1/1
32	PHO	A	409	-	-	8/37/103/103	0/5/6/6
50	NEX	s	623	-	-	7/27/83/83	0/3/3/3
51	LPX	s	625	-	-	13/31/31/31	-
31	CLA	S	605	-	1/1/12/20	10/19/97/115	-
31	CLA	G	614	-	1/1/11/20	10/18/96/115	-
31	CLA	C	505	-	1/1/15/20	14/37/115/115	-
31	CLA	B1	607	-	1/1/15/20	17/37/115/115	-
44	PL9	d1	405	-	-	22/53/73/73	0/1/1/1
53	SPH	y	625	-	-	13/21/21/21	-
41	LHG	d	409	-	-	29/53/53/53	-
47	CHL	g	609	-	4/4/20/26	6/39/137/137	-
31	CLA	b1	608	-	1/1/15/20	24/37/115/115	-
31	CLA	n1	612	-	1/1/11/20	6/13/91/115	-
31	CLA	S1	617	23	1/1/12/20	7/19/97/115	-
31	CLA	y	602	-	1/1/15/20	21/37/115/115	-
47	CHL	y1	601	24	4/4/20/26	2/39/137/137	-
48	LUT	s1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	s1	602	-	1/1/14/20	11/31/109/115	-
33	BCR	a1	411	-	-	13/29/63/63	0/2/2/2
33	BCR	A	411	-	-	13/29/63/63	0/2/2/2
41	LHG	S	624	-	-	28/49/49/53	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	c	514	-	-	12/29/63/63	0/2/2/2
31	CLA	b	604	-	1/1/15/20	18/37/115/115	-
33	BCR	C	514	-	-	10/29/63/63	0/2/2/2
50	NEX	S	622	-	-	12/27/83/83	0/3/3/3
31	CLA	g1	602	-	1/1/15/20	19/37/115/115	-
31	CLA	s	614	-	1/1/13/20	10/25/103/115	-
31	CLA	R1	608	-	1/1/14/20	13/31/109/115	-
31	CLA	R	603	-	1/1/14/20	16/31/109/115	-
31	CLA	Y1	610	-	1/1/15/20	15/37/115/115	-
33	BCR	c1	514	-	-	14/29/63/63	0/2/2/2
31	CLA	b	613	-	1/1/15/20	18/37/115/115	-
56	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
35	LMG	C	521	-	-	20/46/66/70	0/1/1/1
31	CLA	C	501	-	1/1/15/20	16/37/115/115	-
47	CHL	s	608	-	4/4/19/26	3/33/131/137	-
31	CLA	R	610	-	1/1/14/20	15/31/109/115	-
31	CLA	y	608	-	1/1/12/20	6/19/97/115	-
47	CHL	S	601	-	3/3/16/26	5/15/113/137	-
41	LHG	G1	624	-	-	30/53/53/53	-
47	CHL	G	609	-	4/4/20/26	12/39/137/137	-
31	CLA	n	613	-	1/1/15/20	16/37/115/115	-
49	XAT	g	622	-	2/2/12/26	1/31/93/93	0/4/4/4
31	CLA	b1	613	-	1/1/15/20	20/37/115/115	-
38	DGA	c	524	-	-	22/45/45/45	-
47	CHL	y	606	-	4/4/20/26	9/39/137/137	-
31	CLA	C1	512	-	1/1/15/20	19/37/115/115	-
31	CLA	y1	608	-	1/1/12/20	9/19/97/115	-
39	GOL	b	625	-	-	2/4/4/4	-
53	SPH	a1	414	-	-	12/21/21/21	-
31	CLA	b1	609	-	1/1/15/20	12/37/115/115	-
38	DGA	B1	625	-	-	24/45/45/45	-
33	BCR	C	516	-	-	15/29/63/63	0/2/2/2
48	LUT	Y1	621	-	-	2/29/67/67	0/2/2/2
42	LMK	C	527	-	1/1/6/6	12/46/46/60	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	y1	606	-	4/4/20/26	5/39/137/137	-
35	LMG	A	413	-	-	12/43/63/70	0/1/1/1
33	BCR	B	619	-	-	3/29/63/63	0/2/2/2
31	CLA	s	602	-	1/1/14/20	14/31/109/115	-
33	BCR	c1	517	-	-	8/29/63/63	0/2/2/2
32	PHO	a1	408	-	-	5/37/103/103	0/5/6/6
31	CLA	C	506	-	1/1/15/20	23/37/115/115	-
31	CLA	R	602	-	1/1/14/20	12/31/109/115	-
31	CLA	B1	617	-	1/1/15/20	15/37/115/115	-
47	CHL	s1	607	-	3/3/15/26	1/12/110/137	-
40	DGD	C1	519	-	-	21/51/91/95	0/2/2/2
41	LHG	D	409	-	-	32/53/53/53	-
50	NEX	y1	623	-	-	7/27/83/83	0/3/3/3
34	SQD	m1	101	-	-	21/37/57/69	0/1/1/1
31	CLA	c	503	-	1/1/15/20	18/37/115/115	-
31	CLA	S1	611	-	1/1/15/20	18/37/115/115	-
47	CHL	g	608	-	3/3/15/26	3/13/111/137	-
33	BCR	b	619	-	-	9/29/63/63	0/2/2/2
50	NEX	G	623	-	-	4/27/83/83	0/3/3/3
31	CLA	B	602	-	1/1/15/20	21/37/115/115	-
31	CLA	R1	609	-	1/1/14/20	11/31/109/115	-
47	CHL	g1	607	-	4/4/20/26	9/39/137/137	-
35	LMG	w1	201	-	-	16/34/54/70	0/1/1/1
48	LUT	g1	620	-	-	5/29/67/67	0/2/2/2
44	PL9	D1	405	-	-	17/53/73/73	0/1/1/1
31	CLA	c1	508	-	1/1/15/20	15/37/115/115	-
35	LMG	B1	622	-	-	17/39/59/70	0/1/1/1
31	CLA	N	602	-	1/1/15/20	15/37/115/115	-
31	CLA	R	611	-	1/1/11/20	4/15/93/115	-
31	CLA	C	512	-	1/1/15/20	18/37/115/115	-
31	CLA	Y1	613	-	1/1/15/20	21/37/115/115	-
35	LMG	D	411	-	-	9/41/61/70	0/1/1/1
40	DGD	c1	519	-	-	18/51/91/95	0/2/2/2
35	LMG	b	622	-	-	12/39/59/70	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PHO	a1	409	-	-	11/37/103/103	0/5/6/6
49	XAT	R1	621	-	-	2/31/93/93	0/4/4/4
31	CLA	R	613	-	1/1/11/20	8/15/93/115	-
31	CLA	y1	603	-	1/1/15/20	17/37/115/115	-
31	CLA	c	511	-	1/1/15/20	14/37/115/115	-
47	CHL	S1	606	-	3/3/15/26	2/13/111/137	-
31	CLA	r1	609	-	1/1/14/20	13/31/109/115	-
31	CLA	s1	614	-	1/1/13/20	9/25/103/115	-
31	CLA	r	602	-	1/1/14/20	6/31/109/115	-
35	LMG	D1	411	-	-	11/41/61/70	0/1/1/1
47	CHL	S	607	-	4/4/15/26	1/12/110/137	-
31	CLA	g1	614	-	1/1/11/20	11/18/96/115	-
31	CLA	B1	610	-	1/1/15/20	14/37/115/115	-
31	CLA	C1	509	-	1/1/15/20	15/37/115/115	-
41	LHG	l	101	-	-	28/53/53/53	-
48	LUT	r1	620	-	-	6/29/67/67	0/2/2/2
47	CHL	s	607	-	4/4/15/26	1/12/110/137	-
33	BCR	c1	515	-	-	15/29/63/63	0/2/2/2
48	LUT	s	620	-	1/1/12/27	3/29/67/67	0/2/2/2
31	CLA	B	604	-	1/1/15/20	17/37/115/115	-
31	CLA	C1	510	-	1/1/15/20	18/37/115/115	-
34	SQD	a1	412	-	-	18/46/66/69	0/1/1/1
31	CLA	n1	610	-	1/1/15/20	18/37/115/115	-
31	CLA	G	604	-	1/1/11/20	8/18/96/115	-
31	CLA	r1	603	-	1/1/14/20	15/31/109/115	-
31	CLA	S1	604	-	1/1/13/20	10/25/103/115	-
39	GOL	I1	101	-	-	0/4/4/4	-
31	CLA	C1	513	-	1/1/15/20	19/37/115/115	-
31	CLA	n1	603	-	1/1/15/20	15/37/115/115	-
31	CLA	g1	610	-	1/1/15/20	17/37/115/115	-
42	LMK	C1	527	-	2/2/6/6	14/46/46/60	-
46	RRX	H	101	-	1/1/11/25	10/29/65/65	0/2/2/2
31	CLA	Y	602	24	1/1/15/20	21/37/115/115	-
54	4RF	i1	101	-	-	27/59/59/59	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	s1	606	-	3/3/15/26	3/13/111/137	-
31	CLA	R	609	-	1/1/14/20	17/31/109/115	-
32	PHO	a	408	-	-	12/37/103/103	0/5/6/6
49	XAT	n1	622	-	1/1/12/26	5/31/93/93	0/4/4/4
51	LPX	S1	625	-	-	10/31/31/31	-
31	CLA	B1	602	-	1/1/15/20	22/37/115/115	-
31	CLA	C	502	-	1/1/15/20	18/37/115/115	-
42	LMK	c1	527	-	2/2/6/6	13/46/46/60	-
31	CLA	Y	611	-	1/1/15/20	13/37/115/115	-
31	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
48	LUT	n1	620	-	-	4/29/67/67	0/2/2/2
49	XAT	R	621	-	1/1/12/26	14/31/93/93	0/4/4/4
33	BCR	b	618	-	-	10/29/63/63	0/2/2/2
33	BCR	B1	619	-	-	7/29/63/63	0/2/2/2
31	CLA	S	604	-	1/1/13/20	11/25/103/115	-
31	CLA	b1	606	-	1/1/15/20	12/37/115/115	-
37	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
40	DGD	C	520	-	-	13/48/88/95	0/2/2/2
47	CHL	n	609	-	4/4/20/26	10/39/137/137	-
53	SPH	Y1	625	-	-	11/21/21/21	-
49	XAT	Y1	622	-	2/2/12/26	2/31/93/93	0/4/4/4
41	LHG	C	525	-	-	28/51/51/53	-
47	CHL	g1	605	-	4/4/16/26	7/18/116/137	-
31	CLA	c	509	-	1/1/15/20	14/37/115/115	-
35	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
31	CLA	S	602	23	1/1/14/20	13/31/109/115	-
50	NEX	r	623	-	-	8/27/83/83	0/3/3/3
31	CLA	C1	508	-	1/1/15/20	14/37/115/115	-
31	CLA	R1	604	-	1/1/11/20	10/18/96/115	-
31	CLA	b	616	-	1/1/15/20	11/37/115/115	-
47	CHL	R	607	-	3/3/16/26	4/20/118/137	-
49	XAT	N	622	-	1/1/12/26	3/31/93/93	0/4/4/4
31	CLA	c	510	-	1/1/15/20	13/37/115/115	-
52	3PH	t1	101	-	-	28/49/49/49	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	S	606	-	3/3/15/26	1/13/111/137	-
40	DGD	b1	623	-	-	11/32/72/95	0/2/2/2
31	CLA	n1	613	-	1/1/15/20	21/37/115/115	-
31	CLA	B	610	-	1/1/15/20	19/37/115/115	-
31	CLA	c1	503	-	1/1/15/20	19/37/115/115	-
31	CLA	C	507	-	1/1/15/20	18/37/115/115	-
48	LUT	Y	620	-	-	6/29/67/67	0/2/2/2
48	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
31	CLA	y1	604	-	1/1/15/20	17/37/115/115	-
41	LHG	G	630	-	-	30/53/53/53	-
41	LHG	d1	408	-	-	29/48/48/53	-
35	LMG	C1	523	-	-	16/50/70/70	0/1/1/1
33	BCR	C1	515	-	-	11/29/63/63	0/2/2/2
31	CLA	b1	603	-	1/1/15/20	15/37/115/115	-
41	LHG	n1	624	-	-	35/53/53/53	-
31	CLA	S1	605	-	1/1/12/20	8/19/97/115	-
31	CLA	b1	610	-	1/1/15/20	15/37/115/115	-
35	LMG	h1	102	-	-	14/43/63/70	0/1/1/1
31	CLA	b	612	-	1/1/15/20	19/37/115/115	-
31	CLA	d1	402	-	1/1/15/20	17/37/115/115	-
31	CLA	N1	611	-	1/1/11/20	9/18/96/115	-
41	LHG	D	408	-	-	31/48/48/53	-
31	CLA	Y1	612	-	1/1/15/20	13/37/115/115	-
31	CLA	B1	613	-	1/1/15/20	15/37/115/115	-
47	CHL	n	601	-	4/4/20/26	6/39/137/137	-
37	C7Z	b1	620	-	1/1/12/26	15/29/67/67	0/2/2/2
34	SQD	c	626	-	-	19/49/69/69	0/1/1/1
49	XAT	y1	622	-	-	4/31/93/93	0/4/4/4
31	CLA	g	612	-	1/1/10/20	6/11/89/115	-
31	CLA	g1	613	-	1/1/15/20	16/37/115/115	-
35	LMG	a1	413	-	-	14/43/63/70	0/1/1/1
31	CLA	B	611	-	1/1/15/20	8/37/115/115	-
31	CLA	Y	604	-	1/1/15/20	19/37/115/115	-
48	LUT	R	620	-	-	9/29/67/67	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	407	-	1/1/11/20	4/18/96/115	-
31	CLA	B	613	-	1/1/15/20	15/37/115/115	-
31	CLA	s	605	-	1/1/12/20	8/19/97/115	-
34	SQD	b1	621	-	-	18/37/57/69	0/1/1/1
31	CLA	b1	612	-	1/1/15/20	12/37/115/115	-
47	CHL	n1	609	-	4/4/20/26	6/39/137/137	-
50	NEX	r1	622	-	-	9/27/83/83	0/3/3/3
45	HEM	F	101	7,6	-	2/12/54/54	-
47	CHL	g1	608	-	3/3/15/26	3/13/111/137	-
47	CHL	n1	601	20	4/4/20/26	10/39/137/137	-
52	3PH	s	626	-	-	31/49/49/49	-
47	CHL	G1	608	-	3/3/15/26	1/13/111/137	-
31	CLA	r	612	-	1/1/14/20	11/31/109/115	-
31	CLA	a	406	-	1/1/15/20	11/37/115/115	-
47	CHL	Y	609	-	4/4/20/26	9/39/137/137	-
47	CHL	s1	608	-	4/4/19/26	5/33/131/137	-
33	BCR	B	618	-	-	12/29/63/63	0/2/2/2
38	DGA	C	524	-	-	26/45/45/45	-
45	HEM	f	101	7,6	-	2/12/54/54	-
31	CLA	N	611	-	1/1/11/20	10/18/96/115	-
31	CLA	n	603	-	1/1/15/20	26/37/115/115	-
31	CLA	g	611	-	1/1/11/20	5/13/91/115	-
31	CLA	g	603	-	1/1/15/20	16/37/115/115	-
31	CLA	b1	611	-	1/1/15/20	12/37/115/115	-
47	CHL	y1	607	-	4/4/20/26	9/39/137/137	-
31	CLA	r	611	-	1/1/11/20	5/15/93/115	-
49	XAT	G1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
50	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
31	CLA	b	615	-	1/1/15/20	11/37/115/115	-
31	CLA	s	617	-	1/1/12/20	9/19/97/115	-
50	NEX	n	623	-	-	4/27/83/83	0/3/3/3
48	LUT	g	621	-	-	2/29/67/67	0/2/2/2
47	CHL	r1	606	-	3/3/15/26	2/13/111/137	-
33	BCR	C1	516	-	-	15/29/63/63	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	g	610	-	1/1/15/20	13/37/115/115	-
35	LMG	j	101	-	-	14/40/60/70	0/1/1/1
40	DGD	c	520	-	-	15/48/88/95	0/2/2/2
31	CLA	r	613	-	1/1/11/20	8/15/93/115	-
31	CLA	a	405	-	1/1/15/20	15/37/115/115	-
31	CLA	y	611	-	1/1/15/20	18/37/115/115	-
31	CLA	c1	504	-	1/1/15/20	14/37/115/115	-
31	CLA	D	402	-	1/1/15/20	18/37/115/115	-
31	CLA	b	607	-	1/1/15/20	16/37/115/115	-
49	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
47	CHL	N1	608	-	3/3/16/26	5/20/118/137	-
40	DGD	c1	520	-	-	12/48/88/95	0/2/2/2
48	LUT	S1	620	-	-	3/29/67/67	0/2/2/2
31	CLA	y	610	-	1/1/15/20	17/37/115/115	-
31	CLA	R	604	-	1/1/11/20	10/18/96/115	-
48	LUT	Y	621	-	1/1/12/27	2/29/67/67	0/2/2/2
31	CLA	r1	612	-	1/1/14/20	16/31/109/115	-
31	CLA	g1	604	-	1/1/11/20	8/18/96/115	-
31	CLA	R1	603	-	1/1/14/20	12/31/109/115	-
47	CHL	y1	605	-	3/3/16/26	1/15/113/137	-
31	CLA	s	613	-	1/1/13/20	10/25/103/115	-
48	LUT	G	621	-	1/1/12/27	6/29/67/67	0/2/2/2
31	CLA	n1	614	-	1/1/11/20	7/18/96/115	-
47	CHL	S	608	-	4/4/19/26	3/33/131/137	-
31	CLA	b1	615	-	1/1/15/20	21/37/115/115	-
34	SQD	M1	101	-	-	18/37/57/69	0/1/1/1
31	CLA	B	609	-	1/1/15/20	17/37/115/115	-
41	LHG	L1	101	-	-	35/53/53/53	-
31	CLA	y1	610	-	1/1/15/20	13/37/115/115	-
50	NEX	N1	623	-	-	5/27/83/83	0/3/3/3
48	LUT	n	620	-	-	6/29/67/67	0/2/2/2
31	CLA	n	602	-	1/1/15/20	19/37/115/115	-
31	CLA	N1	612	-	1/1/11/20	7/13/91/115	-
31	CLA	Y1	611	-	1/1/15/20	14/37/115/115	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	Y1	603	-	1/1/15/20	19/37/115/115	-
31	CLA	a1	410	-	1/1/14/20	9/31/109/115	-
52	3PH	s1	626	-	-	23/49/49/49	-
31	CLA	C	509	-	1/1/15/20	12/37/115/115	-
48	LUT	n	621	-	1/1/12/27	5/29/67/67	0/2/2/2
40	DGD	C	523	-	-	17/55/95/95	0/2/2/2
31	CLA	N	614	-	1/1/11/20	6/18/96/115	-
31	CLA	c	506	-	1/1/15/20	23/37/115/115	-
47	CHL	n1	607	-	4/4/20/26	5/39/137/137	-
47	CHL	R	606	-	3/3/15/26	5/13/111/137	-
31	CLA	C	510	-	1/1/15/20	17/37/115/115	-
31	CLA	r	609	-	1/1/14/20	17/31/109/115	-
47	CHL	N	608	-	3/3/16/26	7/20/118/137	-
31	CLA	b1	614	-	1/1/15/20	13/37/115/115	-
48	LUT	y	621	-	-	3/29/67/67	0/2/2/2
31	CLA	s1	605	23	1/1/12/20	9/19/97/115	-
31	CLA	S1	610	-	1/1/15/20	20/37/115/115	-
46	RRX	h1	101	-	1/1/11/25	9/29/65/65	0/2/2/2
31	CLA	C	513	-	1/1/15/20	21/37/115/115	-
31	CLA	y	604	-	1/1/15/20	20/37/115/115	-
47	CHL	N	605	-	4/4/20/26	8/39/137/137	-
31	CLA	C	511	-	1/1/15/20	12/37/115/115	-
31	CLA	s1	617	-	1/1/12/20	7/19/97/115	-
47	CHL	G	605	21	3/3/16/26	4/18/116/137	-
31	CLA	s	604	-	1/1/13/20	11/25/103/115	-
31	CLA	g	614	-	1/1/11/20	9/18/96/115	-
50	NEX	g	623	-	-	4/27/83/83	0/3/3/3
31	CLA	B	607	-	1/1/15/20	19/37/115/115	-
31	CLA	y	613	-	1/1/15/20	19/37/115/115	-
31	CLA	y	614	-	1/1/15/20	14/37/115/115	-
48	LUT	Y1	620	-	-	5/29/67/67	0/2/2/2
32	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
31	CLA	y1	611	-	1/1/15/20	12/37/115/115	-
33	BCR	B1	618	-	-	11/29/63/63	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	y1	613	-	1/1/15/20	24/37/115/115	-
48	LUT	N	620	-	-	6/29/67/67	0/2/2/2
31	CLA	Y	614	-	1/1/15/20	11/37/115/115	-
31	CLA	b	606	-	1/1/15/20	13/37/115/115	-
31	CLA	C1	502	-	1/1/15/20	12/37/115/115	-

All (3725) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	101	RRX	C21-C22	66.78	2.24	1.35
56	R1	626	ERG	C1-C10	-23.16	1.10	1.54
56	r1	626	ERG	C1-C10	-22.95	1.10	1.54
56	r1	626	ERG	C10-C9	-20.09	1.28	1.55
56	R1	626	ERG	C10-C9	-19.60	1.29	1.55
37	b	620	C7Z	C25-C26	16.17	1.62	1.34
37	B	620	C7Z	C25-C26	15.97	1.62	1.34
46	h	101	RRX	C26-C25	15.80	1.61	1.34
37	b1	620	C7Z	C25-C26	15.71	1.61	1.34
37	B1	620	C7Z	C25-C26	15.63	1.61	1.34
46	H1	101	RRX	C26-C25	15.32	1.61	1.34
46	h1	101	RRX	C26-C25	15.24	1.60	1.34
37	B	620	C7Z	C5-C6	15.22	1.60	1.34
37	b	620	C7Z	C5-C6	15.20	1.60	1.34
46	H	101	RRX	C26-C25	15.18	1.60	1.34
48	n1	620	LUT	C24-C25	14.92	1.51	1.33
37	B1	620	C7Z	C5-C6	14.92	1.60	1.34
46	h1	101	RRX	C5-C6	14.85	1.60	1.34
46	H1	101	RRX	C5-C6	14.79	1.60	1.34
37	b1	620	C7Z	C5-C6	14.78	1.60	1.34
48	n1	621	LUT	C24-C25	14.73	1.51	1.33
48	N1	620	LUT	C24-C25	14.73	1.51	1.33
46	h	101	RRX	C5-C6	14.72	1.59	1.34
48	s	620	LUT	C24-C25	14.69	1.51	1.33
48	y1	620	LUT	C24-C25	14.65	1.51	1.33
48	S	620	LUT	C24-C25	14.64	1.51	1.33
48	g1	621	LUT	C24-C25	14.64	1.51	1.33
48	g	620	LUT	C24-C25	14.63	1.51	1.33
48	n	621	LUT	C24-C25	14.60	1.51	1.33
48	s1	620	LUT	C24-C25	14.60	1.51	1.33
48	y1	621	LUT	C24-C25	14.59	1.51	1.33
46	H	101	RRX	C5-C6	14.57	1.59	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Y	620	LUT	C24-C25	14.55	1.51	1.33
48	S1	621	LUT	C24-C25	14.55	1.51	1.33
48	r1	620	LUT	C24-C25	14.51	1.51	1.33
48	Y1	621	LUT	C24-C25	14.51	1.51	1.33
48	r	620	LUT	C24-C25	14.51	1.51	1.33
48	g1	620	LUT	C24-C25	14.50	1.51	1.33
48	Y1	620	LUT	C24-C25	14.47	1.51	1.33
48	G1	621	LUT	C24-C25	14.47	1.51	1.33
48	n	620	LUT	C24-C25	14.45	1.51	1.33
48	G	620	LUT	C24-C25	14.44	1.51	1.33
48	N	621	LUT	C24-C25	14.43	1.51	1.33
48	N	620	LUT	C24-C25	14.43	1.51	1.33
48	G1	620	LUT	C24-C25	14.41	1.51	1.33
48	N1	621	LUT	C24-C25	14.40	1.51	1.33
48	g	621	LUT	C24-C25	14.39	1.51	1.33
48	G	621	LUT	C24-C25	14.37	1.51	1.33
48	s	621	LUT	C24-C25	14.35	1.51	1.33
48	S	621	LUT	C24-C25	14.34	1.51	1.33
48	S1	620	LUT	C24-C25	14.31	1.51	1.33
48	y	620	LUT	C24-C25	14.31	1.51	1.33
48	R1	620	LUT	C24-C25	14.31	1.51	1.33
48	s1	621	LUT	C24-C25	14.25	1.50	1.33
48	R	620	LUT	C24-C25	14.21	1.50	1.33
48	y	621	LUT	C24-C25	14.13	1.50	1.33
56	r1	626	ERG	C4-C3	-14.03	1.27	1.52
48	Y	621	LUT	C24-C25	13.93	1.50	1.33
56	r1	626	ERG	C10-C5	-13.86	1.25	1.52
56	R1	626	ERG	C10-C5	-13.82	1.25	1.52
56	R1	626	ERG	C4-C3	-13.54	1.28	1.52
37	B1	620	C7Z	C24-C23	12.43	1.73	1.52
37	b	620	C7Z	C24-C23	11.65	1.72	1.52
37	B	620	C7Z	C24-C23	11.47	1.72	1.52
37	b1	620	C7Z	C24-C23	11.38	1.72	1.52
56	r1	626	ERG	C2-C3	-11.31	1.24	1.51
37	b	620	C7Z	C22-C23	-11.25	1.36	1.52
56	R1	626	ERG	C2-C3	-11.05	1.25	1.51
37	B	620	C7Z	C22-C23	-11.00	1.36	1.52
46	h1	101	RRX	C29-C28	-10.47	1.37	1.52
37	b1	620	C7Z	C22-C23	-10.38	1.37	1.52
37	b	620	C7Z	C2-C3	-10.31	1.37	1.52
37	b1	620	C7Z	C2-C3	-10.28	1.37	1.52
46	H1	101	RRX	C29-C28	-10.28	1.37	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B1	620	C7Z	C2-C3	-10.26	1.37	1.52
37	B	620	C7Z	C2-C3	-10.18	1.37	1.52
46	h	101	RRX	C29-C28	-10.09	1.37	1.52
46	H	101	RRX	C29-C28	-9.92	1.38	1.52
37	B1	620	C7Z	C22-C23	-9.86	1.38	1.52
56	r1	626	ERG	C12-C13	9.16	1.70	1.54
56	R1	626	ERG	C12-C13	9.09	1.70	1.54
56	R1	626	ERG	O1-C3	9.08	1.70	1.43
56	r1	626	ERG	O1-C3	9.02	1.70	1.43
56	R1	626	ERG	C6-C5	8.92	1.54	1.33
56	r1	626	ERG	C6-C5	8.89	1.54	1.33
37	b1	620	C7Z	C4-C3	8.62	1.67	1.52
37	B1	620	C7Z	C4-C3	8.56	1.67	1.52
37	B	620	C7Z	C4-C3	8.51	1.67	1.52
37	b	620	C7Z	C4-C3	8.29	1.66	1.52
50	s1	623	NEX	C10-C9	-8.26	1.24	1.35
46	H	101	RRX	C27-C28	8.05	1.66	1.52
46	h	101	RRX	C27-C28	8.04	1.66	1.52
50	n	623	NEX	C10-C9	-7.91	1.25	1.35
50	n1	623	NEX	C10-C9	-7.91	1.25	1.35
50	y1	623	NEX	C10-C9	-7.85	1.25	1.35
50	r	623	NEX	C10-C9	-7.85	1.25	1.35
46	h1	101	RRX	C27-C28	7.80	1.65	1.52
50	g1	623	NEX	C10-C9	-7.80	1.25	1.35
46	H	101	RRX	C23-C22	7.78	1.62	1.45
50	s1	623	NEX	C14-C13	-7.74	1.25	1.35
50	n	623	NEX	C34-C33	-7.74	1.25	1.35
50	G1	623	NEX	C14-C13	-7.69	1.25	1.35
50	Y	623	NEX	C14-C13	-7.64	1.25	1.35
50	N	623	NEX	C34-C33	-7.64	1.25	1.35
33	D1	404	BCR	C10-C9	7.63	1.45	1.35
46	H1	101	RRX	C27-C28	7.62	1.65	1.52
50	S1	623	NEX	C10-C9	-7.61	1.25	1.35
50	n	623	NEX	C30-C29	-7.57	1.25	1.35
33	d	404	BCR	C10-C9	7.57	1.45	1.35
33	B1	618	BCR	C10-C9	7.56	1.45	1.35
50	g1	623	NEX	C34-C33	-7.56	1.25	1.35
50	N	623	NEX	C14-C13	-7.56	1.25	1.35
50	Y1	623	NEX	C30-C29	-7.55	1.25	1.35
50	s1	623	NEX	C30-C29	-7.55	1.25	1.35
50	N	623	NEX	C10-C9	-7.50	1.25	1.35
50	g	623	NEX	C10-C9	-7.50	1.25	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	n	623	NEX	C14-C13	-7.48	1.25	1.35
50	s	623	NEX	C34-C33	-7.48	1.25	1.35
50	N1	623	NEX	C14-C13	-7.47	1.25	1.35
50	R1	622	NEX	C30-C29	-7.46	1.25	1.35
50	N1	623	NEX	C34-C33	-7.44	1.25	1.35
33	c	516	BCR	C10-C9	7.43	1.45	1.35
33	c1	516	BCR	C10-C9	7.43	1.45	1.35
50	R	622	NEX	C30-C29	-7.43	1.25	1.35
33	C1	517	BCR	C10-C9	7.43	1.45	1.35
50	r	623	NEX	C30-C29	-7.41	1.26	1.35
50	N1	623	NEX	C30-C29	-7.40	1.26	1.35
33	D	404	BCR	C10-C9	7.40	1.45	1.35
50	Y	623	NEX	C30-C29	-7.39	1.26	1.35
50	G	623	NEX	C30-C29	-7.39	1.26	1.35
50	N	623	NEX	C30-C29	-7.37	1.26	1.35
33	c1	515	BCR	C10-C9	7.37	1.45	1.35
50	r1	622	NEX	C34-C33	-7.37	1.26	1.35
50	G1	623	NEX	C30-C29	-7.36	1.26	1.35
50	S1	623	NEX	C14-C13	-7.36	1.26	1.35
50	R	622	NEX	C34-C33	-7.35	1.26	1.35
33	b1	618	BCR	C10-C9	7.35	1.45	1.35
33	C1	515	BCR	C10-C9	7.34	1.45	1.35
33	a1	411	BCR	C10-C9	7.30	1.45	1.35
50	r	623	NEX	C34-C33	-7.29	1.26	1.35
50	S	622	NEX	C34-C33	-7.29	1.26	1.35
50	s	623	NEX	C14-C13	-7.29	1.26	1.35
50	G1	623	NEX	C34-C33	-7.29	1.26	1.35
50	S	622	NEX	C30-C29	-7.28	1.26	1.35
50	G1	623	NEX	C10-C9	-7.28	1.26	1.35
50	r	623	NEX	C14-C13	-7.28	1.26	1.35
50	r1	622	NEX	C14-C13	-7.27	1.26	1.35
50	g	623	NEX	C30-C29	-7.26	1.26	1.35
50	S	622	NEX	C14-C13	-7.24	1.26	1.35
50	g	623	NEX	C14-C13	-7.23	1.26	1.35
50	r1	622	NEX	C30-C29	-7.23	1.26	1.35
50	R1	622	NEX	C14-C13	-7.23	1.26	1.35
50	S1	623	NEX	C30-C29	-7.22	1.26	1.35
50	Y	623	NEX	C10-C9	-7.22	1.26	1.35
50	r1	622	NEX	C10-C9	-7.21	1.26	1.35
50	Y1	623	NEX	C14-C13	-7.20	1.26	1.35
33	b	619	BCR	C10-C9	7.20	1.45	1.35
50	s	623	NEX	C30-C29	-7.19	1.26	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C1	514	BCR	C10-C9	7.19	1.45	1.35
33	C	516	BCR	C10-C9	7.19	1.45	1.35
50	Y	623	NEX	C34-C33	-7.18	1.26	1.35
50	Y1	623	NEX	C34-C33	-7.17	1.26	1.35
33	b	618	BCR	C10-C9	7.16	1.45	1.35
42	C1	527	LMK	O3-C4	7.15	1.44	1.22
50	G	623	NEX	C14-C13	-7.14	1.26	1.35
50	s1	623	NEX	C34-C33	-7.14	1.26	1.35
50	g1	623	NEX	C30-C29	-7.14	1.26	1.35
50	y1	623	NEX	C30-C29	-7.13	1.26	1.35
50	G	623	NEX	C34-C33	-7.13	1.26	1.35
50	n1	623	NEX	C14-C13	-7.12	1.26	1.35
50	s	623	NEX	C10-C9	-7.12	1.26	1.35
50	y1	623	NEX	C34-C33	-7.11	1.26	1.35
50	R1	622	NEX	C34-C33	-7.11	1.26	1.35
42	C	527	LMK	O3-C4	7.11	1.43	1.22
50	y	623	NEX	C10-C9	-7.11	1.26	1.35
33	B1	619	BCR	C10-C9	7.11	1.45	1.35
42	c1	527	LMK	O3-C4	7.09	1.43	1.22
50	G	623	NEX	C10-C9	-7.09	1.26	1.35
50	S1	623	NEX	C34-C33	-7.08	1.26	1.35
50	R	622	NEX	C14-C13	-7.08	1.26	1.35
33	c	514	BCR	C10-C9	7.07	1.45	1.35
42	c	627	LMK	O3-C4	7.07	1.43	1.22
33	b1	619	BCR	C10-C9	7.05	1.45	1.35
50	Y1	623	NEX	C10-C9	-7.05	1.26	1.35
50	y	623	NEX	C34-C33	-7.05	1.26	1.35
50	g1	623	NEX	C14-C13	-7.05	1.26	1.35
33	B	619	BCR	C10-C9	7.03	1.45	1.35
50	g	623	NEX	C34-C33	-7.02	1.26	1.35
50	n1	623	NEX	C30-C29	-7.02	1.26	1.35
50	n1	623	NEX	C34-C33	-7.01	1.26	1.35
50	y	623	NEX	C30-C29	-7.01	1.26	1.35
33	c1	514	BCR	C10-C9	7.00	1.45	1.35
50	y1	623	NEX	C14-C13	-7.00	1.26	1.35
50	N1	623	NEX	C10-C9	-6.99	1.26	1.35
50	R1	622	NEX	C10-C9	-6.97	1.26	1.35
50	y	623	NEX	C14-C13	-6.93	1.26	1.35
33	a	411	BCR	C10-C9	6.89	1.44	1.35
50	s	623	NEX	C35-C15	-6.85	1.18	1.36
33	C	514	BCR	C10-C9	6.84	1.44	1.35
50	n	623	NEX	C35-C15	-6.84	1.18	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d1	404	BCR	C10-C9	6.82	1.44	1.35
33	B	618	BCR	C10-C9	6.80	1.44	1.35
33	c	517	BCR	C10-C9	6.79	1.44	1.35
50	g1	623	NEX	C35-C15	-6.78	1.18	1.36
33	c	515	BCR	C10-C9	6.76	1.44	1.35
33	C	515	BCR	C10-C9	6.76	1.44	1.35
50	r	623	NEX	C35-C15	-6.75	1.18	1.36
50	N	623	NEX	C35-C15	-6.75	1.18	1.36
33	A	411	BCR	C10-C9	6.74	1.44	1.35
50	R	622	NEX	C35-C15	-6.71	1.18	1.36
50	G1	623	NEX	C35-C15	-6.71	1.18	1.36
50	S	622	NEX	C10-C9	-6.71	1.26	1.35
50	s1	623	NEX	C35-C15	-6.70	1.18	1.36
50	N1	623	NEX	C35-C15	-6.70	1.18	1.36
33	C	517	BCR	C10-C9	6.69	1.44	1.35
50	G	623	NEX	C35-C15	-6.68	1.18	1.36
50	S	622	NEX	C35-C15	-6.68	1.18	1.36
50	g	623	NEX	C35-C15	-6.66	1.18	1.36
50	R1	622	NEX	C35-C15	-6.66	1.18	1.36
50	r1	622	NEX	C35-C15	-6.66	1.18	1.36
50	Y	623	NEX	C35-C15	-6.65	1.18	1.36
50	S1	623	NEX	C35-C15	-6.65	1.18	1.36
33	A1	411	BCR	C10-C9	6.62	1.44	1.35
50	n1	623	NEX	C35-C15	-6.61	1.18	1.36
50	Y1	623	NEX	C35-C15	-6.61	1.18	1.36
50	y	623	NEX	C35-C15	-6.60	1.18	1.36
50	r1	622	NEX	C7-C8	6.60	1.43	1.32
50	y1	623	NEX	C35-C15	-6.60	1.18	1.36
50	Y1	623	NEX	C11-C12	-6.56	1.17	1.34
31	r1	612	CLA	MG-NA	6.55	2.21	2.06
31	s1	611	CLA	MG-NA	6.55	2.21	2.06
50	G	623	NEX	C11-C12	-6.53	1.17	1.34
31	c	509	CLA	MG-NA	6.52	2.21	2.06
50	r1	622	NEX	C11-C12	-6.51	1.17	1.34
31	b1	616	CLA	MG-NA	6.49	2.21	2.06
31	s1	613	CLA	MG-NA	6.49	2.21	2.06
31	r	612	CLA	MG-NA	6.49	2.21	2.06
31	R	611	CLA	MG-NA	6.49	2.21	2.06
31	s1	605	CLA	MG-NA	6.48	2.21	2.06
31	b	616	CLA	MG-NA	6.48	2.21	2.06
31	c	513	CLA	MG-NA	6.48	2.21	2.06
31	R1	608	CLA	MG-NA	6.48	2.21	2.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	609	CLA	MG-NA	6.48	2.21	2.06
31	s	605	CLA	MG-NA	6.47	2.21	2.06
31	b1	602	CLA	MG-NA	6.46	2.21	2.06
31	N1	613	CLA	MG-NA	6.46	2.21	2.06
31	n1	612	CLA	MG-NA	6.46	2.21	2.06
31	S1	603	CLA	MG-NA	6.46	2.21	2.06
50	R1	622	NEX	C11-C12	-6.46	1.17	1.34
31	R1	612	CLA	MG-NA	6.45	2.21	2.06
31	B	616	CLA	MG-NA	6.45	2.21	2.06
31	c1	513	CLA	MG-NA	6.45	2.21	2.06
31	g1	614	CLA	MG-NA	6.45	2.21	2.06
31	n	611	CLA	MG-NA	6.45	2.21	2.06
31	r1	608	CLA	MG-NA	6.45	2.21	2.06
31	B1	615	CLA	MG-NA	6.44	2.21	2.06
31	N	611	CLA	MG-NA	6.44	2.21	2.06
31	r	611	CLA	MG-NA	6.44	2.21	2.06
31	g	611	CLA	MG-NA	6.44	2.21	2.06
31	r	603	CLA	MG-NA	6.44	2.21	2.06
31	S	617	CLA	MG-NA	6.43	2.21	2.06
31	g	613	CLA	MG-NA	6.43	2.21	2.06
46	h	101	RRX	C2-C3	-6.43	1.36	1.52
31	R	603	CLA	MG-NA	6.42	2.21	2.06
31	b1	609	CLA	MG-NA	6.42	2.21	2.06
31	C1	512	CLA	MG-NA	6.41	2.21	2.06
31	s	611	CLA	MG-NA	6.41	2.21	2.06
31	g1	603	CLA	MG-NA	6.41	2.21	2.06
31	s	617	CLA	MG-NA	6.41	2.21	2.06
31	g1	612	CLA	MG-NA	6.41	2.21	2.06
50	R	622	NEX	C11-C12	-6.41	1.18	1.34
31	R1	603	CLA	MG-NA	6.41	2.21	2.06
31	s1	603	CLA	MG-NA	6.41	2.21	2.06
31	Y1	608	CLA	MG-NA	6.40	2.21	2.06
31	B	607	CLA	MG-NA	6.40	2.21	2.06
31	s1	609	CLA	MG-NA	6.40	2.21	2.06
31	R	610	CLA	MG-NA	6.40	2.21	2.06
31	R	608	CLA	MG-NA	6.40	2.21	2.06
31	s	603	CLA	MG-NA	6.40	2.21	2.06
31	c1	505	CLA	MG-NA	6.40	2.21	2.06
50	N	623	NEX	C11-C12	-6.40	1.18	1.34
31	B	602	CLA	MG-NA	6.40	2.21	2.06
31	G	613	CLA	MG-NA	6.40	2.21	2.06
31	n1	614	CLA	MG-NA	6.40	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	612	CLA	MG-NA	6.39	2.21	2.06
31	R	612	CLA	MG-NA	6.39	2.21	2.06
31	b1	615	CLA	MG-NA	6.39	2.21	2.06
31	b	602	CLA	MG-NA	6.39	2.21	2.06
31	G1	614	CLA	MG-NA	6.38	2.21	2.06
31	B	609	CLA	MG-NA	6.38	2.21	2.06
31	r	613	CLA	MG-NA	6.38	2.21	2.06
31	g	612	CLA	MG-NA	6.38	2.21	2.06
31	c1	512	CLA	MG-NA	6.38	2.21	2.06
31	R	613	CLA	MG-NA	6.37	2.21	2.06
31	s	613	CLA	MG-NA	6.37	2.21	2.06
31	b	608	CLA	MG-NA	6.37	2.21	2.06
31	s	610	CLA	MG-NA	6.37	2.21	2.06
50	N1	623	NEX	C11-C12	-6.37	1.18	1.34
46	h1	101	RRX	C2-C3	-6.37	1.36	1.52
31	S	612	CLA	MG-NA	6.37	2.21	2.06
31	R	602	CLA	MG-NA	6.37	2.21	2.06
31	r	610	CLA	MG-NA	6.37	2.21	2.06
31	n	614	CLA	MG-NA	6.37	2.21	2.06
31	g	604	CLA	MG-NA	6.37	2.21	2.06
31	s1	604	CLA	MG-NA	6.37	2.21	2.06
31	c	503	CLA	MG-NA	6.36	2.21	2.06
31	y	608	CLA	MG-NA	6.36	2.21	2.06
31	g	614	CLA	MG-NA	6.36	2.21	2.06
31	r	602	CLA	MG-NA	6.36	2.21	2.06
31	B	604	CLA	MG-NA	6.36	2.21	2.06
31	C	512	CLA	MG-NA	6.36	2.21	2.06
31	Y	608	CLA	MG-NA	6.36	2.21	2.06
31	S	602	CLA	MG-NA	6.35	2.21	2.06
31	d1	402	CLA	MG-NA	6.35	2.21	2.06
31	G1	612	CLA	MG-NA	6.35	2.21	2.06
31	N	612	CLA	MG-NA	6.35	2.21	2.06
31	Y	611	CLA	MG-NA	6.35	2.21	2.06
31	b	609	CLA	MG-NA	6.35	2.21	2.06
31	N	613	CLA	MG-NA	6.35	2.21	2.06
31	n	602	CLA	MG-NA	6.35	2.21	2.06
46	H1	101	RRX	C2-C3	-6.35	1.36	1.52
46	H	101	RRX	C2-C3	-6.35	1.36	1.52
31	b1	614	CLA	MG-NA	6.35	2.21	2.06
31	c	512	CLA	MG-NA	6.35	2.21	2.06
31	C	503	CLA	MG-NA	6.35	2.21	2.06
31	B1	609	CLA	MG-NA	6.35	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	612	CLA	MG-NA	6.34	2.21	2.06
31	d	403	CLA	MG-NA	6.34	2.21	2.06
31	B	610	CLA	MG-NA	6.34	2.21	2.06
31	S	609	CLA	MG-NA	6.34	2.21	2.06
31	r1	602	CLA	MG-NA	6.34	2.21	2.06
31	b1	603	CLA	MG-NA	6.34	2.21	2.06
31	r1	603	CLA	MG-NA	6.34	2.21	2.06
31	B	611	CLA	MG-NA	6.34	2.21	2.06
31	N1	611	CLA	MG-NA	6.33	2.21	2.06
31	c1	501	CLA	MG-NA	6.33	2.21	2.06
31	n1	613	CLA	MG-NA	6.33	2.21	2.06
31	y1	608	CLA	MG-NA	6.33	2.21	2.06
31	y1	611	CLA	MG-NA	6.33	2.21	2.06
31	G	611	CLA	MG-NA	6.33	2.21	2.06
31	g1	604	CLA	MG-NA	6.33	2.21	2.06
31	B1	602	CLA	MG-NA	6.33	2.21	2.06
31	s1	617	CLA	MG-NA	6.33	2.21	2.06
31	Y1	603	CLA	MG-NA	6.33	2.21	2.06
31	c1	507	CLA	MG-NA	6.33	2.21	2.06
31	c1	506	CLA	MG-NA	6.33	2.21	2.06
31	b	611	CLA	MG-NA	6.33	2.21	2.06
31	S1	609	CLA	MG-NA	6.33	2.21	2.06
31	g1	611	CLA	MG-NA	6.33	2.21	2.06
31	D	403	CLA	MG-NA	6.32	2.21	2.06
31	b1	617	CLA	MG-NA	6.32	2.21	2.06
31	C	507	CLA	MG-NA	6.32	2.21	2.06
31	R1	602	CLA	MG-NA	6.32	2.21	2.06
31	N	614	CLA	MG-NA	6.32	2.21	2.06
31	S	603	CLA	MG-NA	6.32	2.21	2.06
31	n	612	CLA	MG-NA	6.32	2.21	2.06
31	C	511	CLA	MG-NA	6.32	2.21	2.06
31	G1	604	CLA	MG-NA	6.32	2.21	2.06
31	c1	509	CLA	MG-NA	6.32	2.21	2.06
50	R	622	NEX	C31-C32	-6.31	1.18	1.34
31	s1	614	CLA	MG-NA	6.31	2.21	2.06
31	b	604	CLA	MG-NA	6.31	2.21	2.06
31	B1	608	CLA	MG-NA	6.31	2.21	2.06
31	r	608	CLA	MG-NA	6.31	2.21	2.06
31	b1	608	CLA	MG-NA	6.31	2.21	2.06
50	s1	623	NEX	C11-C12	-6.31	1.18	1.34
31	S	611	CLA	MG-NA	6.31	2.21	2.06
31	n	613	CLA	MG-NA	6.31	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	610	CLA	MG-NA	6.31	2.21	2.06
31	C1	503	CLA	MG-NA	6.31	2.21	2.06
31	g1	610	CLA	MG-NA	6.31	2.21	2.06
31	S	605	CLA	MG-NA	6.31	2.21	2.06
31	A1	407	CLA	MG-NA	6.31	2.21	2.06
31	Y	614	CLA	MG-NA	6.30	2.21	2.06
50	n	623	NEX	C31-C32	-6.30	1.18	1.34
31	y	612	CLA	MG-NA	6.30	2.21	2.06
31	C1	502	CLA	MG-NA	6.30	2.21	2.06
31	n1	603	CLA	MG-NA	6.30	2.21	2.06
31	S	613	CLA	MG-NA	6.30	2.21	2.06
31	G	604	CLA	MG-NA	6.29	2.21	2.06
31	S1	604	CLA	MG-NA	6.29	2.21	2.06
31	y1	612	CLA	MG-NA	6.29	2.21	2.06
31	A1	405	CLA	MG-NA	6.29	2.21	2.06
31	N1	612	CLA	MG-NA	6.29	2.21	2.06
31	S1	605	CLA	MG-NA	6.29	2.21	2.06
31	Y	612	CLA	MG-NA	6.29	2.21	2.06
31	Y	613	CLA	MG-NA	6.29	2.21	2.06
31	Y1	602	CLA	MG-NA	6.29	2.21	2.06
31	S1	617	CLA	MG-NA	6.29	2.21	2.06
50	G1	623	NEX	C11-C12	-6.29	1.18	1.34
31	a1	407	CLA	MG-NA	6.28	2.21	2.06
31	r1	609	CLA	MG-NA	6.28	2.21	2.06
31	r	609	CLA	MG-NA	6.28	2.21	2.06
31	B1	604	CLA	MG-NA	6.28	2.21	2.06
31	B1	613	CLA	MG-NA	6.28	2.21	2.06
31	b1	611	CLA	MG-NA	6.28	2.21	2.06
31	Y1	614	CLA	MG-NA	6.28	2.21	2.06
50	s1	623	NEX	C31-C32	-6.28	1.18	1.34
31	B	612	CLA	MG-NA	6.28	2.21	2.06
50	Y1	623	NEX	C31-C32	-6.28	1.18	1.34
31	R	609	CLA	MG-NA	6.28	2.21	2.06
31	c1	511	CLA	MG-NA	6.28	2.21	2.06
31	n1	604	CLA	MG-NA	6.28	2.21	2.06
31	y1	614	CLA	MG-NA	6.28	2.21	2.06
31	N	604	CLA	MG-NA	6.27	2.21	2.06
31	c	506	CLA	MG-NA	6.27	2.21	2.06
31	y	610	CLA	MG-NA	6.27	2.21	2.06
31	a1	410	CLA	MG-NA	6.27	2.21	2.06
31	R1	609	CLA	MG-NA	6.27	2.21	2.06
31	s1	610	CLA	MG-NA	6.27	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a1	405	CLA	MG-NA	6.27	2.21	2.06
31	y1	604	CLA	MG-NA	6.27	2.21	2.06
31	b	615	CLA	MG-NA	6.27	2.21	2.06
31	S	604	CLA	MG-NA	6.27	2.21	2.06
31	G1	603	CLA	MG-NA	6.27	2.21	2.06
31	c	507	CLA	MG-NA	6.27	2.21	2.06
31	r1	610	CLA	MG-NA	6.27	2.21	2.06
31	a	407	CLA	MG-NA	6.26	2.21	2.06
31	n1	611	CLA	MG-NA	6.26	2.21	2.06
31	B1	607	CLA	MG-NA	6.26	2.21	2.06
31	y	614	CLA	MG-NA	6.26	2.21	2.06
31	c	511	CLA	MG-NA	6.26	2.21	2.06
31	G1	613	CLA	MG-NA	6.26	2.21	2.06
31	S1	614	CLA	MG-NA	6.26	2.21	2.06
31	R1	610	CLA	MG-NA	6.26	2.21	2.06
31	C1	511	CLA	MG-NA	6.26	2.21	2.06
31	B1	611	CLA	MG-NA	6.26	2.21	2.06
50	N1	623	NEX	C31-C32	-6.25	1.18	1.34
31	R	604	CLA	MG-NA	6.25	2.21	2.06
31	c1	510	CLA	MG-NA	6.25	2.21	2.06
31	B	608	CLA	MG-NA	6.25	2.21	2.06
50	r	623	NEX	C31-C32	-6.25	1.18	1.34
31	B1	614	CLA	MG-NA	6.25	2.21	2.06
31	Y1	612	CLA	MG-NA	6.25	2.21	2.06
50	n	623	NEX	C11-C12	-6.25	1.18	1.34
31	D1	403	CLA	MG-NA	6.25	2.21	2.06
31	c	502	CLA	MG-NA	6.25	2.21	2.06
31	g	603	CLA	MG-NA	6.25	2.21	2.06
31	S1	612	CLA	MG-NA	6.25	2.21	2.06
50	N	623	NEX	C31-C32	-6.25	1.18	1.34
31	b1	610	CLA	MG-NA	6.24	2.21	2.06
31	g1	613	CLA	MG-NA	6.24	2.21	2.06
31	A	407	CLA	MG-NA	6.24	2.21	2.06
31	a	410	CLA	MG-NA	6.24	2.21	2.06
31	g	602	CLA	MG-NA	6.24	2.21	2.06
31	G	614	CLA	MG-NA	6.24	2.21	2.06
31	G1	611	CLA	MG-NA	6.24	2.21	2.06
31	b	603	CLA	MG-NA	6.23	2.21	2.06
31	g1	602	CLA	MG-NA	6.23	2.21	2.06
31	d1	403	CLA	MG-NA	6.23	2.21	2.06
31	b1	606	CLA	MG-NA	6.23	2.21	2.06
31	B	606	CLA	MG-NA	6.23	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R1	604	CLA	MG-NA	6.23	2.21	2.06
31	b	607	CLA	MG-NA	6.23	2.21	2.06
50	g1	623	NEX	C31-C32	-6.23	1.18	1.34
31	B	614	CLA	MG-NA	6.23	2.21	2.06
50	r	623	NEX	C11-C12	-6.23	1.18	1.34
31	y	611	CLA	MG-NA	6.23	2.21	2.06
31	B	613	CLA	MG-NA	6.22	2.21	2.06
50	S1	623	NEX	C31-C32	-6.22	1.18	1.34
31	S1	613	CLA	MG-NA	6.22	2.21	2.06
50	s	623	NEX	C31-C32	-6.22	1.18	1.34
31	y1	603	CLA	MG-NA	6.22	2.21	2.06
31	C	510	CLA	MG-NA	6.22	2.21	2.06
31	C	502	CLA	MG-NA	6.22	2.21	2.06
31	Y1	604	CLA	MG-NA	6.22	2.21	2.06
31	B1	616	CLA	MG-NA	6.22	2.21	2.06
31	c	505	CLA	MG-NA	6.22	2.21	2.06
31	c1	503	CLA	MG-NA	6.22	2.21	2.06
50	R1	622	NEX	C31-C32	-6.21	1.18	1.34
31	y1	602	CLA	MG-NA	6.21	2.21	2.06
31	A1	406	CLA	MG-NA	6.21	2.21	2.06
50	S1	623	NEX	C11-C12	-6.21	1.18	1.34
31	C1	501	CLA	MG-NA	6.21	2.21	2.06
31	C	506	CLA	MG-NA	6.21	2.21	2.06
31	S1	611	CLA	MG-NA	6.21	2.21	2.06
50	g	623	NEX	C11-C12	-6.21	1.18	1.34
31	G	603	CLA	MG-NA	6.21	2.21	2.06
31	s	604	CLA	MG-NA	6.20	2.21	2.06
31	Y1	611	CLA	MG-NA	6.20	2.21	2.06
31	B1	610	CLA	MG-NA	6.20	2.21	2.06
31	B	603	CLA	MG-NA	6.20	2.21	2.06
31	c1	504	CLA	MG-NA	6.20	2.21	2.06
31	S	614	CLA	MG-NA	6.20	2.21	2.06
31	n1	602	CLA	MG-NA	6.20	2.21	2.06
50	G1	623	NEX	C31-C32	-6.20	1.18	1.34
31	s1	612	CLA	MG-NA	6.20	2.21	2.06
31	N	602	CLA	MG-NA	6.20	2.21	2.06
31	b	617	CLA	MG-NA	6.19	2.21	2.06
50	S	622	NEX	C11-C12	-6.19	1.18	1.34
31	B1	606	CLA	MG-NA	6.19	2.21	2.06
31	C1	507	CLA	MG-NA	6.19	2.21	2.06
31	N1	603	CLA	MG-NA	6.19	2.21	2.06
50	G	623	NEX	C31-C32	-6.19	1.18	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	603	CLA	MG-NA	6.19	2.21	2.06
31	S1	602	CLA	MG-NA	6.19	2.21	2.06
31	b1	613	CLA	MG-NA	6.19	2.21	2.06
31	b	612	CLA	MG-NA	6.19	2.21	2.06
31	N1	614	CLA	MG-NA	6.19	2.21	2.06
31	A	410	CLA	MG-NA	6.19	2.21	2.06
31	Y	603	CLA	MG-NA	6.19	2.21	2.06
31	B1	617	CLA	MG-NA	6.19	2.21	2.06
31	G	602	CLA	MG-NA	6.19	2.21	2.06
31	c	501	CLA	MG-NA	6.19	2.21	2.06
31	B1	603	CLA	MG-NA	6.18	2.21	2.06
31	y	613	CLA	MG-NA	6.18	2.21	2.06
31	r	604	CLA	MG-NA	6.18	2.20	2.06
31	S1	610	CLA	MG-NA	6.18	2.20	2.06
31	C1	513	CLA	MG-NA	6.17	2.20	2.06
31	G1	602	CLA	MG-NA	6.17	2.20	2.06
50	r1	622	NEX	C31-C32	-6.17	1.18	1.34
31	C	509	CLA	MG-NA	6.17	2.20	2.06
50	Y	623	NEX	C31-C32	-6.17	1.18	1.34
31	g	610	CLA	MG-NA	6.17	2.20	2.06
31	N1	604	CLA	MG-NA	6.16	2.20	2.06
31	y1	613	CLA	MG-NA	6.16	2.20	2.06
31	B	605	CLA	MG-NA	6.16	2.20	2.06
31	Y	604	CLA	MG-NA	6.16	2.20	2.06
33	c1	517	BCR	C10-C9	6.16	1.43	1.35
31	C	501	CLA	MG-NA	6.16	2.20	2.06
50	g	623	NEX	C31-C32	-6.16	1.18	1.34
31	A1	410	CLA	MG-NA	6.15	2.20	2.06
31	b1	604	CLA	MG-NA	6.15	2.20	2.06
31	d	402	CLA	MG-NA	6.15	2.20	2.06
31	c	510	CLA	MG-NA	6.15	2.20	2.06
31	r1	604	CLA	MG-NA	6.15	2.20	2.06
31	B	617	CLA	MG-NA	6.15	2.20	2.06
31	b	605	CLA	MG-NA	6.15	2.20	2.06
31	C	513	CLA	MG-NA	6.14	2.20	2.06
31	S	610	CLA	MG-NA	6.14	2.20	2.06
46	H	101	RRX	C1-C6	-6.14	1.45	1.53
31	C1	505	CLA	MG-NA	6.14	2.20	2.06
31	Y1	613	CLA	MG-NA	6.14	2.20	2.06
31	y	604	CLA	MG-NA	6.14	2.20	2.06
31	A	406	CLA	MG-NA	6.14	2.20	2.06
50	s	623	NEX	C11-C12	-6.13	1.18	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	610	CLA	MG-NA	6.13	2.20	2.06
31	B1	612	CLA	MG-NA	6.12	2.20	2.06
31	n	603	CLA	MG-NA	6.12	2.20	2.06
50	y1	623	NEX	C31-C32	-6.12	1.18	1.34
31	a	406	CLA	MG-NA	6.12	2.20	2.06
50	g	623	NEX	C7-C8	6.12	1.42	1.32
31	b1	607	CLA	MG-NA	6.12	2.20	2.06
31	b	614	CLA	MG-NA	6.12	2.20	2.06
31	c1	502	CLA	MG-NA	6.12	2.20	2.06
31	n1	610	CLA	MG-NA	6.11	2.20	2.06
31	y1	610	CLA	MG-NA	6.11	2.20	2.06
31	a	405	CLA	MG-NA	6.11	2.20	2.06
31	C1	506	CLA	MG-NA	6.11	2.20	2.06
56	r1	626	ERG	C16-C17	-6.11	1.41	1.54
31	b	610	CLA	MG-NA	6.10	2.20	2.06
31	Y	602	CLA	MG-NA	6.10	2.20	2.06
50	S	622	NEX	C31-C32	-6.09	1.18	1.34
31	c	504	CLA	MG-NA	6.09	2.20	2.06
31	s	614	CLA	MG-NA	6.09	2.20	2.06
31	s1	602	CLA	MG-NA	6.09	2.20	2.06
31	C	505	CLA	MG-NA	6.09	2.20	2.06
31	C1	510	CLA	MG-NA	6.08	2.20	2.06
31	y	603	CLA	MG-NA	6.08	2.20	2.06
50	G	623	NEX	C7-C8	6.08	1.42	1.32
31	c1	508	CLA	MG-NA	6.07	2.20	2.06
31	B	615	CLA	MG-NA	6.07	2.20	2.06
56	R1	626	ERG	C16-C17	-6.07	1.41	1.54
31	b1	612	CLA	MG-NA	6.07	2.20	2.06
31	C	508	CLA	MG-NA	6.07	2.20	2.06
50	y1	623	NEX	C11-C12	-6.07	1.18	1.34
31	b	606	CLA	MG-NA	6.06	2.20	2.06
31	B1	605	CLA	MG-NA	6.06	2.20	2.06
50	y	623	NEX	C11-C12	-6.05	1.19	1.34
31	a1	406	CLA	MG-NA	6.05	2.20	2.06
33	c1	517	BCR	C24-C23	6.05	1.51	1.33
31	c	508	CLA	MG-NA	6.04	2.20	2.06
31	C1	509	CLA	MG-NA	6.04	2.20	2.06
50	y	623	NEX	C31-C32	-6.04	1.19	1.34
31	G1	610	CLA	MG-NA	6.03	2.20	2.06
50	g1	623	NEX	C11-C12	-6.03	1.19	1.34
31	D	402	CLA	MG-NA	6.02	2.20	2.06
31	C1	504	CLA	MG-NA	6.01	2.20	2.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	405	CLA	MG-NA	6.01	2.20	2.06
33	b	619	BCR	C24-C23	6.01	1.51	1.33
31	N1	602	CLA	MG-NA	6.00	2.20	2.06
31	b	613	CLA	MG-NA	5.99	2.20	2.06
50	Y	623	NEX	C11-C12	-5.99	1.19	1.34
31	s	602	CLA	MG-NA	5.99	2.20	2.06
50	N	623	NEX	C7-C8	5.98	1.41	1.32
46	H1	101	RRX	C1-C6	-5.97	1.45	1.53
31	C1	508	CLA	MG-NA	5.97	2.20	2.06
31	D1	402	CLA	MG-NA	5.95	2.20	2.06
50	n1	623	NEX	C31-C32	-5.95	1.19	1.34
31	b1	605	CLA	MG-NA	5.95	2.20	2.06
50	n1	623	NEX	C11-C12	-5.94	1.19	1.34
31	n	610	CLA	MG-NA	5.94	2.20	2.06
46	H	101	RRX	C37-C22	5.93	1.63	1.50
31	C	504	CLA	MG-NA	5.93	2.20	2.06
31	G	610	CLA	MG-NA	5.92	2.20	2.06
31	y	602	CLA	MG-NA	5.91	2.20	2.06
33	D	404	BCR	C24-C23	5.90	1.50	1.33
31	n	604	CLA	MG-NA	5.89	2.20	2.06
31	N1	610	CLA	MG-NA	5.89	2.20	2.06
31	Y1	610	CLA	MG-NA	5.88	2.20	2.06
37	B1	620	C7Z	C12-C13	5.87	1.58	1.45
33	B1	618	BCR	C24-C23	5.86	1.50	1.33
33	C1	516	BCR	C24-C23	5.85	1.50	1.33
33	c	514	BCR	C24-C23	5.85	1.50	1.33
33	B1	619	BCR	C24-C23	5.84	1.50	1.33
46	h	101	RRX	C1-C6	-5.84	1.45	1.53
33	d1	404	BCR	C24-C23	5.81	1.50	1.33
33	c	517	BCR	C24-C23	5.80	1.50	1.33
37	B	620	C7Z	C12-C13	5.79	1.58	1.45
33	b1	619	BCR	C24-C23	5.79	1.50	1.33
33	D1	404	BCR	C24-C23	5.77	1.50	1.33
33	b1	618	BCR	C24-C23	5.76	1.50	1.33
33	C	517	BCR	C24-C23	5.75	1.50	1.33
37	b1	620	C7Z	C12-C13	5.74	1.58	1.45
33	d	404	BCR	C24-C23	5.74	1.50	1.33
33	C1	514	BCR	C24-C23	5.73	1.50	1.33
33	C1	515	BCR	C24-C23	5.73	1.50	1.33
33	b	618	BCR	C24-C23	5.73	1.50	1.33
33	B	619	BCR	C24-C23	5.73	1.50	1.33
33	c1	515	BCR	C24-C23	5.72	1.50	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c1	516	BCR	C24-C23	5.72	1.50	1.33
33	A1	411	BCR	C24-C23	5.70	1.50	1.33
50	R	622	NEX	C10-C9	-5.68	1.28	1.35
37	b1	620	C7Z	C1-C6	-5.68	1.46	1.53
33	C	516	BCR	C24-C23	5.65	1.50	1.33
33	a	411	BCR	C24-C23	5.65	1.50	1.33
37	b	620	C7Z	C12-C13	5.63	1.58	1.45
50	N1	623	NEX	C7-C8	5.63	1.41	1.32
33	C	514	BCR	C24-C23	5.63	1.50	1.33
33	A	411	BCR	C24-C23	5.60	1.50	1.33
33	C1	517	BCR	C24-C23	5.58	1.49	1.33
33	a1	411	BCR	C24-C23	5.58	1.49	1.33
50	y	623	NEX	C7-C8	5.58	1.41	1.32
33	C	515	BCR	C24-C23	5.58	1.49	1.33
33	c1	514	BCR	C24-C23	5.56	1.49	1.33
50	y1	623	NEX	C7-C8	5.55	1.41	1.32
33	c	516	BCR	C24-C23	5.54	1.49	1.33
33	B	618	BCR	C24-C23	5.54	1.49	1.33
50	G1	623	NEX	C7-C8	5.52	1.41	1.32
50	Y1	623	NEX	C7-C8	5.48	1.41	1.32
50	g1	623	NEX	C7-C8	5.47	1.41	1.32
46	h	101	RRX	C30-C25	-5.46	1.46	1.53
37	B1	620	C7Z	C1-C6	-5.42	1.46	1.53
46	h1	101	RRX	C19-C18	5.40	1.57	1.45
46	H	101	RRX	C20-C21	5.40	1.60	1.43
56	R1	626	ERG	C13-C14	-5.37	1.47	1.56
33	c	515	BCR	C24-C23	5.36	1.49	1.33
33	c	517	BCR	C11-C12	-5.35	1.20	1.34
46	h1	101	RRX	C1-C6	-5.34	1.46	1.53
33	C1	517	BCR	C11-C12	-5.34	1.20	1.34
33	c	515	BCR	C11-C12	-5.32	1.20	1.34
37	b	620	C7Z	C28-C29	5.32	1.57	1.45
46	H	101	RRX	C30-C25	-5.31	1.46	1.53
46	h1	101	RRX	C8-C9	5.31	1.57	1.45
33	B	618	BCR	C11-C12	-5.30	1.20	1.34
33	C	517	BCR	C11-C12	-5.30	1.20	1.34
33	a	411	BCR	C11-C12	-5.29	1.20	1.34
50	S	622	NEX	C7-C8	5.29	1.40	1.32
46	h1	101	RRX	C2-C1	5.26	1.66	1.54
50	Y	623	NEX	C7-C8	5.26	1.40	1.32
50	Y1	623	NEX	C28-C29	-5.26	1.34	1.45
56	R1	626	ERG	C1-C2	5.25	1.64	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	411	BCR	C11-C12	-5.24	1.21	1.34
33	C	514	BCR	C11-C12	-5.24	1.21	1.34
37	B	620	C7Z	C28-C29	5.24	1.57	1.45
50	N1	623	NEX	C28-C29	-5.24	1.34	1.45
33	c1	514	BCR	C11-C12	-5.23	1.21	1.34
50	N	623	NEX	C28-C29	-5.23	1.34	1.45
50	r1	622	NEX	C28-C29	-5.23	1.34	1.45
33	c	514	BCR	C11-C12	-5.23	1.21	1.34
33	c1	515	BCR	C11-C12	-5.23	1.21	1.34
50	s	623	NEX	C28-C29	-5.23	1.34	1.45
50	r	623	NEX	C28-C29	-5.22	1.34	1.45
33	B	619	BCR	C11-C12	-5.21	1.21	1.34
50	R	622	NEX	C28-C29	-5.20	1.34	1.45
50	s1	623	NEX	C28-C29	-5.19	1.34	1.45
33	C	515	BCR	C11-C12	-5.19	1.21	1.34
37	B1	620	C7Z	C28-C29	5.19	1.57	1.45
50	n	623	NEX	C7-C8	5.19	1.40	1.32
46	H	101	RRX	C19-C18	5.19	1.57	1.45
50	S1	623	NEX	C28-C29	-5.19	1.34	1.45
33	B1	619	BCR	C11-C12	-5.18	1.21	1.34
33	C1	516	BCR	C10-C9	5.18	1.42	1.35
50	G	623	NEX	C28-C29	-5.18	1.34	1.45
33	C	516	BCR	C11-C12	-5.17	1.21	1.34
33	d1	404	BCR	C11-C12	-5.16	1.21	1.34
50	g	623	NEX	C28-C29	-5.16	1.34	1.45
50	R1	622	NEX	C28-C29	-5.15	1.34	1.45
50	Y	623	NEX	C28-C29	-5.15	1.34	1.45
56	r1	626	ERG	C13-C14	-5.15	1.47	1.56
50	n	623	NEX	C28-C29	-5.13	1.34	1.45
46	H1	101	RRX	C2-C1	5.13	1.66	1.54
33	C1	514	BCR	C11-C12	-5.13	1.21	1.34
50	S1	623	NEX	C7-C8	5.13	1.40	1.32
50	y1	623	NEX	C28-C29	-5.12	1.34	1.45
33	a1	411	BCR	C11-C12	-5.12	1.21	1.34
50	R	622	NEX	C7-C8	5.12	1.40	1.32
33	A1	411	BCR	C11-C12	-5.11	1.21	1.34
33	b	618	BCR	C11-C12	-5.11	1.21	1.34
33	b1	619	BCR	C11-C12	-5.11	1.21	1.34
33	b	619	BCR	C11-C12	-5.10	1.21	1.34
37	B	620	C7Z	C1-C6	-5.10	1.46	1.53
50	S	622	NEX	C28-C29	-5.10	1.35	1.45
33	c1	517	BCR	C11-C12	-5.08	1.21	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	n1	623	NEX	C7-C8	5.07	1.40	1.32
50	g1	623	NEX	C28-C29	-5.07	1.35	1.45
46	H	101	RRX	C2-C1	5.07	1.65	1.54
50	y	623	NEX	C28-C29	-5.06	1.35	1.45
46	h	101	RRX	C2-C1	5.04	1.65	1.54
46	h1	101	RRX	C30-C25	-5.04	1.46	1.53
33	c1	516	BCR	C11-C12	-5.04	1.21	1.34
56	r1	626	ERG	C1-C2	5.04	1.64	1.53
50	G1	623	NEX	C28-C29	-5.03	1.35	1.45
46	H1	101	RRX	C30-C25	-5.02	1.46	1.53
46	h	101	RRX	C19-C18	5.02	1.56	1.45
33	C1	515	BCR	C11-C12	-5.02	1.21	1.34
33	b1	618	BCR	C11-C12	-5.01	1.21	1.34
50	r	623	NEX	C7-C8	4.99	1.40	1.32
33	D	404	BCR	C11-C12	-4.98	1.21	1.34
50	n1	623	NEX	C28-C29	-4.98	1.35	1.45
37	b1	620	C7Z	C28-C29	4.97	1.56	1.45
37	b1	620	C7Z	C24-C25	-4.97	1.43	1.51
33	D1	404	BCR	C11-C12	-4.97	1.21	1.34
33	c	516	BCR	C11-C12	-4.96	1.21	1.34
50	s1	623	NEX	C7-C8	4.95	1.40	1.32
46	H1	101	RRX	C19-C18	4.95	1.56	1.45
37	b	620	C7Z	C1-C6	-4.94	1.47	1.53
50	R1	622	NEX	C7-C8	4.93	1.40	1.32
37	B	620	C7Z	C32-C33	4.91	1.56	1.45
33	B1	618	BCR	C11-C12	-4.89	1.22	1.34
37	b	620	C7Z	C32-C33	4.86	1.56	1.45
56	r1	626	ERG	C12-C11	-4.86	1.43	1.53
45	f	101	HEM	C3C-C2C	-4.86	1.33	1.40
37	B1	620	C7Z	C32-C33	4.82	1.56	1.45
33	C1	516	BCR	C11-C12	-4.82	1.22	1.34
33	d	404	BCR	C11-C12	-4.80	1.22	1.34
56	r1	626	ERG	C7-C6	-4.79	1.27	1.41
37	b1	620	C7Z	C32-C33	4.77	1.56	1.45
45	F	101	HEM	C3C-C2C	-4.76	1.33	1.40
46	H1	101	RRX	C8-C9	4.76	1.56	1.45
46	h	101	RRX	C8-C9	4.76	1.56	1.45
56	R1	626	ERG	C7-C6	-4.75	1.27	1.41
46	H	101	RRX	C8-C9	4.74	1.56	1.45
44	d1	405	PL9	C7-C3	-4.73	1.46	1.51
56	R1	626	ERG	C12-C11	-4.68	1.43	1.53
37	B	620	C7Z	C24-C25	-4.63	1.43	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	h1	101	RRX	C12-C13	4.60	1.55	1.45
37	b	620	C7Z	C24-C25	-4.60	1.43	1.51
50	s	623	NEX	C7-C8	4.58	1.39	1.32
46	h	101	RRX	C27-C26	-4.51	1.44	1.51
33	A1	411	BCR	C16-C17	-4.50	1.29	1.43
37	B1	620	C7Z	C31-C30	4.50	1.57	1.43
33	c	515	BCR	C16-C17	-4.50	1.29	1.43
31	b	609	CLA	MG-ND	-4.49	1.96	2.05
37	B	620	C7Z	C31-C30	4.48	1.57	1.43
37	b	620	C7Z	C31-C30	4.48	1.57	1.43
37	b	620	C7Z	C4-C5	-4.48	1.44	1.51
56	R1	626	ERG	C13-C17	4.44	1.63	1.55
33	C1	517	BCR	C16-C17	-4.43	1.29	1.43
46	H	101	RRX	C27-C26	-4.43	1.44	1.51
37	B	620	C7Z	C8-C9	4.42	1.55	1.45
46	H1	101	RRX	C27-C26	-4.42	1.44	1.51
33	a1	411	BCR	C16-C17	-4.40	1.29	1.43
56	r1	626	ERG	C13-C17	4.40	1.63	1.55
33	A	411	BCR	C16-C17	-4.39	1.29	1.43
33	c	517	BCR	C16-C17	-4.38	1.29	1.43
46	H1	101	RRX	C23-C22	4.38	1.55	1.45
46	h1	101	RRX	C27-C26	-4.37	1.44	1.51
33	C	515	BCR	C16-C17	-4.36	1.29	1.43
33	a	411	BCR	C16-C17	-4.36	1.29	1.43
37	B1	620	C7Z	C24-C25	-4.36	1.44	1.51
33	C	516	BCR	C16-C17	-4.36	1.29	1.43
37	b1	620	C7Z	C31-C30	4.36	1.56	1.43
40	C1	519	DGD	O1G-C1A	4.35	1.46	1.33
46	H	101	RRX	C3-C4	4.34	1.66	1.52
40	C	523	DGD	O1G-C1A	4.34	1.46	1.33
40	c1	518	DGD	O1G-C1A	4.34	1.46	1.33
40	C	518	DGD	O1G-C1A	4.34	1.46	1.33
46	h1	101	RRX	C23-C22	4.33	1.55	1.45
46	H1	101	RRX	C3-C4	4.32	1.66	1.52
46	H	101	RRX	C12-C13	4.32	1.55	1.45
33	d1	404	BCR	C16-C17	-4.32	1.30	1.43
44	D	405	PL9	C7-C3	-4.32	1.46	1.51
33	C	517	BCR	C16-C17	-4.32	1.30	1.43
46	h1	101	RRX	C3-C4	4.32	1.66	1.52
37	b	620	C7Z	C8-C9	4.31	1.55	1.45
37	B1	620	C7Z	C8-C9	4.30	1.55	1.45
37	b1	620	C7Z	C8-C9	4.30	1.55	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	514	BCR	C16-C17	-4.28	1.30	1.43
40	c1	520	DGD	O1G-C1A	4.28	1.45	1.33
37	B	620	C7Z	C11-C10	4.28	1.56	1.43
37	B1	620	C7Z	C11-C10	4.28	1.56	1.43
40	c	518	DGD	O1G-C1A	4.28	1.45	1.33
33	B	619	BCR	C16-C17	-4.28	1.30	1.43
33	b	618	BCR	C16-C17	-4.27	1.30	1.43
31	B	609	CLA	MG-ND	-4.27	1.97	2.05
46	h	101	RRX	C12-C13	4.27	1.55	1.45
46	h	101	RRX	C3-C4	4.26	1.65	1.52
37	b1	620	C7Z	C4-C5	-4.26	1.44	1.51
37	B	620	C7Z	C4-C5	-4.25	1.44	1.51
31	B1	609	CLA	MG-ND	-4.25	1.97	2.05
40	c	523	DGD	O1G-C1A	4.24	1.45	1.33
40	b1	623	DGD	O1G-C1A	4.24	1.45	1.33
31	b1	609	CLA	MG-ND	-4.23	1.97	2.05
40	C	519	DGD	O1G-C1A	4.23	1.45	1.33
46	H1	101	RRX	C12-C13	4.23	1.55	1.45
37	b1	620	C7Z	C11-C10	4.23	1.56	1.43
40	C	520	DGD	O1G-C1A	4.22	1.45	1.33
40	B1	623	DGD	O1G-C1A	4.22	1.45	1.33
33	B1	619	BCR	C16-C17	-4.22	1.30	1.43
33	b1	619	BCR	C16-C17	-4.22	1.30	1.43
33	c1	514	BCR	C16-C17	-4.21	1.30	1.43
40	C1	520	DGD	O1G-C1A	4.21	1.45	1.33
40	c1	519	DGD	O1G-C1A	4.20	1.45	1.33
33	C1	515	BCR	C16-C17	-4.19	1.30	1.43
46	h1	101	RRX	C20-C21	4.19	1.56	1.43
33	C1	514	BCR	C16-C17	-4.19	1.30	1.43
31	N1	604	CLA	MG-ND	-4.18	1.97	2.05
40	C1	518	DGD	O1G-C1A	4.18	1.45	1.33
33	B	618	BCR	C16-C17	-4.18	1.30	1.43
56	R1	626	ERG	C16-C15	4.18	1.65	1.54
33	b1	618	BCR	C16-C17	-4.17	1.30	1.43
31	D1	402	CLA	MG-ND	-4.17	1.97	2.05
33	c1	516	BCR	C16-C17	-4.16	1.30	1.43
33	d	404	BCR	C16-C17	-4.16	1.30	1.43
31	C	507	CLA	MG-ND	-4.16	1.97	2.05
31	c	505	CLA	MG-ND	-4.16	1.97	2.05
31	C1	510	CLA	MG-ND	-4.14	1.97	2.05
40	c	520	DGD	O1G-C1A	4.14	1.45	1.33
31	B	604	CLA	MG-ND	-4.13	1.97	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	514	BCR	C16-C17	-4.13	1.30	1.43
37	b	620	C7Z	C11-C10	4.12	1.56	1.43
33	c1	517	BCR	C16-C17	-4.12	1.30	1.43
31	B	617	CLA	MG-ND	-4.11	1.97	2.05
33	c	516	BCR	C16-C17	-4.11	1.30	1.43
31	b1	617	CLA	MG-ND	-4.10	1.97	2.05
33	b	619	BCR	C16-C17	-4.10	1.30	1.43
31	b	613	CLA	MG-ND	-4.09	1.97	2.05
31	B	612	CLA	MG-ND	-4.09	1.97	2.05
31	c1	505	CLA	MG-ND	-4.09	1.97	2.05
31	c	506	CLA	MG-ND	-4.08	1.97	2.05
31	r1	603	CLA	MG-ND	-4.08	1.97	2.05
37	B1	620	C7Z	C4-C5	-4.07	1.44	1.51
31	Y1	614	CLA	MG-ND	-4.07	1.97	2.05
31	C1	506	CLA	MG-ND	-4.07	1.97	2.05
31	G1	604	CLA	MG-ND	-4.07	1.97	2.05
33	B1	618	BCR	C16-C17	-4.06	1.30	1.43
31	B1	604	CLA	MG-ND	-4.06	1.97	2.05
31	A1	405	CLA	MG-ND	-4.06	1.97	2.05
33	D	404	BCR	C16-C17	-4.06	1.30	1.43
31	s1	611	CLA	MG-ND	-4.06	1.97	2.05
31	C	505	CLA	MG-ND	-4.05	1.97	2.05
33	D1	404	BCR	C16-C17	-4.05	1.30	1.43
31	C	508	CLA	MG-ND	-4.05	1.97	2.05
31	c	508	CLA	C1C-NC	-4.04	1.31	1.37
31	S1	610	CLA	MG-ND	-4.04	1.97	2.05
31	b	612	CLA	MG-ND	-4.04	1.97	2.05
46	h1	101	RRX	C15-C14	4.04	1.56	1.43
31	c1	510	CLA	MG-ND	-4.04	1.97	2.05
42	C1	527	LMK	O2-C4	4.04	1.43	1.30
31	d1	402	CLA	MG-ND	-4.03	1.97	2.05
31	S	612	CLA	MG-ND	-4.03	1.97	2.05
31	A	410	CLA	MG-ND	-4.03	1.97	2.05
31	B	607	CLA	MG-ND	-4.02	1.97	2.05
31	S	603	CLA	MG-ND	-4.02	1.97	2.05
31	C	506	CLA	MG-ND	-4.02	1.97	2.05
31	B	613	CLA	MG-ND	-4.02	1.97	2.05
31	b	604	CLA	MG-ND	-4.02	1.97	2.05
31	b1	615	CLA	MG-ND	-4.02	1.97	2.05
31	y	604	CLA	MG-ND	-4.01	1.97	2.05
31	c	509	CLA	MG-ND	-4.01	1.97	2.05
31	y1	611	CLA	MG-ND	-4.01	1.97	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	c	627	LMK	O2-C4	4.01	1.43	1.30
56	r1	626	ERG	C16-C15	4.00	1.65	1.54
31	d	402	CLA	MG-ND	-4.00	1.97	2.05
31	c1	512	CLA	MG-ND	-4.00	1.97	2.05
42	C	527	LMK	O2-C4	4.00	1.43	1.30
45	f1	101	HEM	C3C-CAC	4.00	1.56	1.47
31	S	614	CLA	MG-ND	-4.00	1.97	2.05
31	S1	611	CLA	MG-ND	-4.00	1.97	2.05
31	Y1	608	CLA	MG-ND	-3.99	1.97	2.05
31	S	610	CLA	MG-ND	-3.99	1.97	2.05
31	b	617	CLA	MG-ND	-3.99	1.97	2.05
31	C1	502	CLA	MG-ND	-3.99	1.97	2.05
31	S1	605	CLA	MG-ND	-3.99	1.97	2.05
31	a	410	CLA	MG-ND	-3.99	1.97	2.05
31	c	513	CLA	MG-ND	-3.98	1.97	2.05
31	d	403	CLA	MG-ND	-3.98	1.97	2.05
33	C1	516	BCR	C16-C17	-3.98	1.31	1.43
31	N1	613	CLA	MG-ND	-3.98	1.97	2.05
31	R1	603	CLA	MG-ND	-3.98	1.97	2.05
31	c	502	CLA	MG-ND	-3.97	1.97	2.05
31	b1	612	CLA	MG-ND	-3.97	1.97	2.05
31	B1	615	CLA	MG-ND	-3.97	1.97	2.05
31	S1	604	CLA	MG-ND	-3.97	1.97	2.05
31	b	605	CLA	MG-ND	-3.97	1.97	2.05
31	B1	613	CLA	MG-ND	-3.97	1.97	2.05
31	C1	505	CLA	MG-ND	-3.96	1.97	2.05
31	N	610	CLA	MG-ND	-3.96	1.97	2.05
31	c	512	CLA	MG-ND	-3.96	1.97	2.05
31	s	613	CLA	MG-ND	-3.95	1.97	2.05
31	C1	503	CLA	MG-ND	-3.95	1.97	2.05
31	B1	607	CLA	MG-ND	-3.95	1.98	2.05
33	c1	515	BCR	C16-C17	-3.95	1.31	1.43
31	s1	614	CLA	MG-ND	-3.95	1.98	2.05
31	N	612	CLA	MG-ND	-3.95	1.98	2.05
31	R	604	CLA	MG-ND	-3.95	1.98	2.05
31	N	602	CLA	MG-ND	-3.95	1.98	2.05
31	B1	606	CLA	MG-ND	-3.95	1.98	2.05
31	Y	611	CLA	MG-ND	-3.95	1.98	2.05
31	S1	617	CLA	MG-ND	-3.94	1.98	2.05
31	G1	612	CLA	MG-ND	-3.94	1.98	2.05
31	B	610	CLA	MG-ND	-3.94	1.98	2.05
31	S	611	CLA	MG-ND	-3.94	1.98	2.05

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S1	613	CLA	MG-ND	-3.94	1.98	2.05
31	C	509	CLA	MG-ND	-3.94	1.98	2.05
31	s	614	CLA	MG-ND	-3.94	1.98	2.05
31	y	612	CLA	MG-ND	-3.94	1.98	2.05
31	A	407	CLA	MG-ND	-3.93	1.98	2.05
31	b	616	CLA	MG-ND	-3.93	1.98	2.05
31	C	503	CLA	MG-ND	-3.93	1.98	2.05
31	a	407	CLA	MG-ND	-3.93	1.98	2.05
31	a	405	CLA	MG-ND	-3.93	1.98	2.05
31	b	607	CLA	MG-ND	-3.93	1.98	2.05
31	G1	614	CLA	MG-ND	-3.93	1.98	2.05
37	b1	620	C7Z	C22-C21	3.93	1.67	1.54
31	b1	603	CLA	MG-ND	-3.93	1.98	2.05
31	C1	507	CLA	MG-ND	-3.92	1.98	2.05
31	C1	508	CLA	MG-ND	-3.92	1.98	2.05
31	b1	610	CLA	MG-ND	-3.92	1.98	2.05
31	b1	613	CLA	MG-ND	-3.92	1.98	2.05
31	c1	507	CLA	MG-ND	-3.92	1.98	2.05
31	s	605	CLA	MG-ND	-3.92	1.98	2.05
31	A1	410	CLA	MG-ND	-3.92	1.98	2.05
40	c	519	DGD	O1G-C1A	3.92	1.44	1.33
31	c	504	CLA	MG-ND	-3.92	1.98	2.05
31	A	405	CLA	MG-ND	-3.92	1.98	2.05
31	b	611	CLA	MG-ND	-3.92	1.98	2.05
31	N1	610	CLA	MG-ND	-3.92	1.98	2.05
31	b	603	CLA	MG-ND	-3.92	1.98	2.05
31	b	606	CLA	MG-ND	-3.92	1.98	2.05
46	h	101	RRX	C20-C21	3.92	1.55	1.43
31	b1	614	CLA	MG-ND	-3.91	1.98	2.05
31	c	511	CLA	MG-ND	-3.91	1.98	2.05
31	Y	613	CLA	MG-ND	-3.91	1.98	2.05
31	g	611	CLA	MG-ND	-3.91	1.98	2.05
31	G1	603	CLA	MG-ND	-3.91	1.98	2.05
31	c1	506	CLA	MG-ND	-3.91	1.98	2.05
31	Y1	603	CLA	MG-ND	-3.91	1.98	2.05
31	c	507	CLA	MG-ND	-3.91	1.98	2.05
31	g1	604	CLA	MG-ND	-3.91	1.98	2.05
31	n1	604	CLA	MG-ND	-3.90	1.98	2.05
31	B1	603	CLA	MG-ND	-3.90	1.98	2.05
31	B1	608	CLA	MG-ND	-3.90	1.98	2.05
31	Y1	613	CLA	MG-ND	-3.90	1.98	2.05
31	Y1	612	CLA	MG-ND	-3.90	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r1	608	CLA	MG-ND	-3.90	1.98	2.05
42	c1	527	LMK	O2-C4	3.90	1.43	1.30
31	Y	614	CLA	MG-ND	-3.90	1.98	2.05
31	B	605	CLA	MG-ND	-3.90	1.98	2.05
31	Y	612	CLA	MG-ND	-3.90	1.98	2.05
31	c	508	CLA	MG-ND	-3.90	1.98	2.05
31	B1	617	CLA	MG-ND	-3.90	1.98	2.05
31	r	603	CLA	MG-ND	-3.90	1.98	2.05
31	n	613	CLA	MG-ND	-3.90	1.98	2.05
31	b1	606	CLA	MG-ND	-3.90	1.98	2.05
31	c	503	CLA	MG-ND	-3.89	1.98	2.05
31	R	609	CLA	MG-ND	-3.89	1.98	2.05
31	S	613	CLA	MG-ND	-3.89	1.98	2.05
31	s	602	CLA	MG-ND	-3.89	1.98	2.05
46	H1	101	RRX	C20-C21	3.88	1.55	1.43
31	b	610	CLA	MG-ND	-3.88	1.98	2.05
31	n	612	CLA	MG-ND	-3.88	1.98	2.05
31	g1	602	CLA	MG-ND	-3.88	1.98	2.05
31	Y1	611	CLA	MG-ND	-3.88	1.98	2.05
31	g	604	CLA	MG-ND	-3.88	1.98	2.05
31	n1	613	CLA	MG-ND	-3.88	1.98	2.05
31	s1	605	CLA	MG-ND	-3.88	1.98	2.05
31	G	611	CLA	MG-ND	-3.88	1.98	2.05
31	N	603	CLA	MG-ND	-3.87	1.98	2.05
31	D	402	CLA	MG-ND	-3.87	1.98	2.05
31	y1	612	CLA	MG-ND	-3.87	1.98	2.05
31	y	610	CLA	MG-ND	-3.87	1.98	2.05
31	s1	610	CLA	MG-ND	-3.87	1.98	2.05
31	a	406	CLA	MG-ND	-3.87	1.98	2.05
31	b	605	CLA	C1C-NC	-3.86	1.32	1.37
31	G1	602	CLA	MG-ND	-3.86	1.98	2.05
31	c1	504	CLA	MG-ND	-3.86	1.98	2.05
46	h	101	RRX	C23-C22	3.86	1.54	1.45
31	B	615	CLA	MG-ND	-3.86	1.98	2.05
31	C	508	CLA	C1C-NC	-3.86	1.32	1.37
37	B1	620	C7Z	C22-C21	3.86	1.66	1.54
31	B	608	CLA	MG-ND	-3.86	1.98	2.05
31	g	603	CLA	MG-ND	-3.86	1.98	2.05
31	G	612	CLA	MG-ND	-3.86	1.98	2.05
31	C1	501	CLA	MG-ND	-3.86	1.98	2.05
31	N1	611	CLA	MG-ND	-3.86	1.98	2.05
31	C	511	CLA	MG-ND	-3.86	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	614	CLA	MG-ND	-3.86	1.98	2.05
31	G	604	CLA	MG-ND	-3.85	1.98	2.05
31	a1	410	CLA	MG-ND	-3.85	1.98	2.05
31	S1	603	CLA	MG-ND	-3.85	1.98	2.05
31	Y1	602	CLA	MG-ND	-3.85	1.98	2.05
31	N1	612	CLA	MG-ND	-3.85	1.98	2.05
37	B	620	C7Z	C27-C26	3.85	1.58	1.45
31	D1	403	CLA	MG-ND	-3.85	1.98	2.05
31	A1	406	CLA	MG-ND	-3.85	1.98	2.05
31	A	406	CLA	MG-ND	-3.85	1.98	2.05
31	C1	504	CLA	MG-ND	-3.85	1.98	2.05
31	r1	609	CLA	MG-ND	-3.85	1.98	2.05
31	b1	605	CLA	C1C-NC	-3.85	1.32	1.37
31	Y	608	CLA	MG-ND	-3.85	1.98	2.05
31	C	501	CLA	MG-ND	-3.85	1.98	2.05
31	c1	511	CLA	MG-ND	-3.84	1.98	2.05
31	n	611	CLA	MG-ND	-3.84	1.98	2.05
31	Y	604	CLA	MG-ND	-3.84	1.98	2.05
31	C1	509	CLA	MG-ND	-3.84	1.98	2.05
31	b1	605	CLA	MG-ND	-3.83	1.98	2.05
31	R	603	CLA	MG-ND	-3.83	1.98	2.05
31	c	510	CLA	MG-ND	-3.83	1.98	2.05
31	s	603	CLA	MG-ND	-3.83	1.98	2.05
31	r1	612	CLA	MG-ND	-3.83	1.98	2.05
31	S1	614	CLA	MG-ND	-3.83	1.98	2.05
31	B	611	CLA	MG-ND	-3.83	1.98	2.05
31	r	604	CLA	MG-ND	-3.83	1.98	2.05
31	a1	407	CLA	MG-ND	-3.83	1.98	2.05
31	y1	610	CLA	MG-ND	-3.83	1.98	2.05
31	r1	610	CLA	MG-ND	-3.83	1.98	2.05
31	b	615	CLA	MG-ND	-3.83	1.98	2.05
31	y	608	CLA	MG-ND	-3.82	1.98	2.05
31	B	606	CLA	MG-ND	-3.82	1.98	2.05
31	g	613	CLA	MG-ND	-3.82	1.98	2.05
31	s	611	CLA	MG-ND	-3.82	1.98	2.05
31	s1	613	CLA	MG-ND	-3.82	1.98	2.05
31	G1	611	CLA	MG-ND	-3.82	1.98	2.05
37	b1	620	C7Z	C15-C14	3.82	1.55	1.43
31	B1	610	CLA	MG-ND	-3.82	1.98	2.05
31	C1	511	CLA	MG-ND	-3.82	1.98	2.05
31	C	513	CLA	MG-ND	-3.82	1.98	2.05
31	b1	612	CLA	C1C-NC	-3.82	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B1	620	C7Z	C15-C14	3.82	1.55	1.43
31	Y1	610	CLA	C1C-NC	-3.82	1.32	1.37
31	c1	508	CLA	MG-ND	-3.81	1.98	2.05
31	C	512	CLA	MG-ND	-3.81	1.98	2.05
31	N	614	CLA	MG-ND	-3.81	1.98	2.05
31	n	603	CLA	MG-ND	-3.81	1.98	2.05
31	n	610	CLA	MG-ND	-3.81	1.98	2.05
31	B1	605	CLA	MG-ND	-3.81	1.98	2.05
31	Y1	610	CLA	MG-ND	-3.81	1.98	2.05
31	d1	403	CLA	MG-ND	-3.81	1.98	2.05
31	B	603	CLA	MG-ND	-3.81	1.98	2.05
31	N	604	CLA	MG-ND	-3.81	1.98	2.05
31	r	612	CLA	MG-ND	-3.81	1.98	2.05
31	Y	603	CLA	MG-ND	-3.81	1.98	2.05
31	y	611	CLA	MG-ND	-3.81	1.98	2.05
31	y	613	CLA	MG-ND	-3.81	1.98	2.05
37	B	620	C7Z	C15-C14	3.81	1.55	1.43
31	S	609	CLA	MG-ND	-3.81	1.98	2.05
31	S1	612	CLA	MG-ND	-3.81	1.98	2.05
31	G	613	CLA	MG-ND	-3.80	1.98	2.05
31	n1	611	CLA	MG-ND	-3.80	1.98	2.05
31	a1	405	CLA	MG-ND	-3.80	1.98	2.05
31	B	602	CLA	MG-ND	-3.80	1.98	2.05
31	c1	503	CLA	MG-ND	-3.80	1.98	2.05
31	s1	603	CLA	MG-ND	-3.80	1.98	2.05
31	G	602	CLA	MG-ND	-3.80	1.98	2.05
31	g1	614	CLA	MG-ND	-3.80	1.98	2.05
31	G	610	CLA	MG-ND	-3.80	1.98	2.05
31	R1	609	CLA	MG-ND	-3.80	1.98	2.05
46	H	101	RRX	C15-C14	3.80	1.55	1.43
31	s1	612	CLA	MG-ND	-3.80	1.98	2.05
31	B	616	CLA	MG-ND	-3.80	1.98	2.05
31	S	604	CLA	MG-ND	-3.80	1.98	2.05
31	s	609	CLA	MG-ND	-3.79	1.98	2.05
31	r	609	CLA	MG-ND	-3.79	1.98	2.05
31	N1	603	CLA	MG-ND	-3.79	1.98	2.05
31	N	613	CLA	MG-ND	-3.79	1.98	2.05
31	b	614	CLA	MG-ND	-3.79	1.98	2.05
31	R1	608	CLA	MG-ND	-3.79	1.98	2.05
31	c	501	CLA	MG-ND	-3.79	1.98	2.05
31	s	604	CLA	MG-ND	-3.79	1.98	2.05
31	g1	612	CLA	MG-ND	-3.79	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	403	CLA	MG-ND	-3.79	1.98	2.05
31	g	614	CLA	MG-ND	-3.79	1.98	2.05
31	S	617	CLA	MG-ND	-3.79	1.98	2.05
31	B1	611	CLA	MG-ND	-3.79	1.98	2.05
45	F	101	HEM	C3C-CAC	3.79	1.55	1.47
31	b	617	CLA	C1C-NC	-3.78	1.32	1.37
31	r1	604	CLA	MG-ND	-3.78	1.98	2.05
31	N	611	CLA	MG-ND	-3.78	1.98	2.05
31	b1	608	CLA	MG-ND	-3.78	1.98	2.05
31	Y	610	CLA	MG-ND	-3.78	1.98	2.05
31	y1	608	CLA	MG-ND	-3.78	1.98	2.05
31	B1	602	CLA	MG-ND	-3.78	1.98	2.05
31	S1	609	CLA	MG-ND	-3.78	1.98	2.05
31	b1	604	CLA	MG-ND	-3.78	1.98	2.05
31	y1	604	CLA	MG-ND	-3.78	1.98	2.05
31	r	610	CLA	MG-ND	-3.78	1.98	2.05
31	C	504	CLA	MG-ND	-3.77	1.98	2.05
31	b1	602	CLA	MG-ND	-3.77	1.98	2.05
31	S1	602	CLA	MG-ND	-3.77	1.98	2.05
31	c1	513	CLA	MG-ND	-3.77	1.98	2.05
31	b1	611	CLA	MG-ND	-3.77	1.98	2.05
31	g	612	CLA	MG-ND	-3.77	1.98	2.05
31	y1	602	CLA	MG-ND	-3.77	1.98	2.05
45	f	101	HEM	C3C-CAC	3.77	1.55	1.47
31	n1	612	CLA	MG-ND	-3.77	1.98	2.05
31	r	602	CLA	MG-ND	-3.77	1.98	2.05
31	s1	602	CLA	MG-ND	-3.77	1.98	2.05
44	d	405	PL9	C7-C3	-3.77	1.47	1.51
31	B1	612	CLA	MG-ND	-3.76	1.98	2.05
31	b	608	CLA	MG-ND	-3.76	1.98	2.05
31	B1	616	CLA	MG-ND	-3.76	1.98	2.05
31	s1	604	CLA	MG-ND	-3.76	1.98	2.05
31	B1	614	CLA	MG-ND	-3.76	1.98	2.05
31	y1	614	CLA	MG-ND	-3.76	1.98	2.05
45	F1	101	HEM	C3C-CAC	3.76	1.55	1.47
46	h	101	RRX	C15-C14	3.76	1.55	1.43
31	R	611	CLA	MG-ND	-3.76	1.98	2.05
31	b1	616	CLA	MG-ND	-3.76	1.98	2.05
37	B1	620	C7Z	C35-C34	3.76	1.55	1.43
31	r	611	CLA	MG-ND	-3.76	1.98	2.05
31	C1	512	CLA	MG-ND	-3.76	1.98	2.05
31	c1	502	CLA	MG-ND	-3.76	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b1	607	CLA	MG-ND	-3.75	1.98	2.05
31	a1	406	CLA	MG-ND	-3.75	1.98	2.05
31	C1	513	CLA	MG-ND	-3.75	1.98	2.05
31	R1	604	CLA	MG-ND	-3.75	1.98	2.05
31	R	602	CLA	MG-ND	-3.75	1.98	2.05
31	S	605	CLA	MG-ND	-3.75	1.98	2.05
31	N1	602	CLA	MG-ND	-3.75	1.98	2.05
37	B	620	C7Z	C22-C21	3.75	1.66	1.54
50	R	622	NEX	C18-C5	-3.75	1.46	1.52
31	n1	610	CLA	MG-ND	-3.74	1.98	2.05
31	S	602	CLA	MG-ND	-3.74	1.98	2.05
31	G1	613	CLA	MG-ND	-3.74	1.98	2.05
31	y1	613	CLA	MG-ND	-3.74	1.98	2.05
37	b	620	C7Z	C15-C14	3.74	1.55	1.43
31	n1	614	CLA	MG-ND	-3.74	1.98	2.05
37	b	620	C7Z	C27-C26	3.74	1.58	1.45
31	R	613	CLA	MG-ND	-3.74	1.98	2.05
31	C	510	CLA	MG-ND	-3.74	1.98	2.05
31	s1	609	CLA	MG-ND	-3.74	1.98	2.05
37	B1	620	C7Z	C27-C26	3.74	1.58	1.45
31	y	603	CLA	MG-ND	-3.74	1.98	2.05
31	n1	602	CLA	MG-ND	-3.74	1.98	2.05
31	g1	613	CLA	MG-ND	-3.74	1.98	2.05
31	D1	402	CLA	C1C-NC	-3.73	1.32	1.37
31	s	610	CLA	MG-ND	-3.73	1.98	2.05
31	n1	603	CLA	MG-ND	-3.73	1.98	2.05
31	C	502	CLA	MG-ND	-3.73	1.98	2.05
31	n	614	CLA	MG-ND	-3.73	1.98	2.05
31	N1	614	CLA	MG-ND	-3.73	1.98	2.05
31	r	613	CLA	MG-ND	-3.73	1.98	2.05
31	y1	603	CLA	MG-ND	-3.73	1.98	2.05
31	Y1	604	CLA	MG-ND	-3.72	1.98	2.05
31	g	602	CLA	MG-ND	-3.72	1.98	2.05
31	R	608	CLA	MG-ND	-3.72	1.98	2.05
31	y	602	CLA	MG-ND	-3.72	1.98	2.05
31	Y	602	CLA	MG-ND	-3.72	1.98	2.05
46	H1	101	RRX	C15-C14	3.71	1.54	1.43
31	c	506	CLA	C1C-NC	-3.71	1.32	1.37
31	n	604	CLA	MG-ND	-3.71	1.98	2.05
31	s	617	CLA	MG-ND	-3.71	1.98	2.05
31	r1	602	CLA	MG-ND	-3.71	1.98	2.05
31	R1	602	CLA	MG-ND	-3.71	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	602	CLA	MG-ND	-3.71	1.98	2.05
31	r	608	CLA	MG-ND	-3.71	1.98	2.05
31	c1	501	CLA	MG-ND	-3.71	1.98	2.05
31	s1	617	CLA	MG-ND	-3.70	1.98	2.05
31	B	614	CLA	MG-ND	-3.70	1.98	2.05
31	R1	612	CLA	MG-ND	-3.70	1.98	2.05
38	b1	625	DGA	OG2-CB1	3.70	1.44	1.34
31	G1	610	CLA	MG-ND	-3.70	1.98	2.05
31	g1	610	CLA	MG-ND	-3.70	1.98	2.05
31	Y	610	CLA	C1C-NC	-3.69	1.32	1.37
31	G	603	CLA	MG-ND	-3.69	1.98	2.05
37	B	620	C7Z	C35-C34	3.69	1.54	1.43
45	F1	101	HEM	C3C-C2C	-3.69	1.35	1.40
37	b	620	C7Z	C2-C1	3.68	1.66	1.54
31	B1	617	CLA	C1C-NC	-3.68	1.32	1.37
44	d	405	PL9	C3-C4	-3.67	1.43	1.49
37	b	620	C7Z	C22-C21	3.67	1.66	1.54
31	R	610	CLA	MG-ND	-3.67	1.98	2.05
31	N1	610	CLA	C1C-NC	-3.67	1.32	1.37
31	g1	603	CLA	MG-ND	-3.67	1.98	2.05
31	n	610	CLA	C1C-NC	-3.66	1.32	1.37
31	G	614	CLA	MG-ND	-3.66	1.98	2.05
31	R1	610	CLA	MG-ND	-3.65	1.98	2.05
31	A1	407	CLA	MG-ND	-3.65	1.98	2.05
31	g	610	CLA	MG-ND	-3.65	1.98	2.05
31	s	612	CLA	MG-ND	-3.65	1.98	2.05
31	n	602	CLA	MG-ND	-3.65	1.98	2.05
31	D	402	CLA	C1C-NC	-3.64	1.32	1.37
31	b	613	CLA	C1C-NC	-3.64	1.32	1.37
37	B	620	C7Z	C2-C1	3.63	1.66	1.54
31	g1	611	CLA	MG-ND	-3.63	1.98	2.05
31	B1	616	CLA	C1C-NC	-3.63	1.32	1.37
37	b	620	C7Z	C35-C34	3.62	1.54	1.43
38	b	623	DGA	OG2-CB1	3.62	1.44	1.34
31	a	406	CLA	C1C-NC	-3.62	1.32	1.37
38	B	625	DGA	OG2-CB1	3.62	1.44	1.34
31	R	612	CLA	MG-ND	-3.61	1.98	2.05
31	c1	502	CLA	C1C-NC	-3.61	1.32	1.37
31	S1	610	CLA	C1C-NC	-3.60	1.32	1.37
37	b1	620	C7Z	C27-C26	3.60	1.57	1.45
38	B1	625	DGA	OG2-CB1	3.60	1.44	1.34
37	b1	620	C7Z	C35-C34	3.60	1.54	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	617	CLA	C1C-NC	-3.59	1.32	1.37
31	s	602	CLA	C1C-NC	-3.59	1.32	1.37
37	b1	620	C7Z	C2-C1	3.58	1.66	1.54
31	B	605	CLA	C1C-NC	-3.58	1.32	1.37
31	b	612	CLA	C1C-NC	-3.57	1.32	1.37
46	h1	101	RRX	C11-C10	3.56	1.54	1.43
31	b1	617	CLA	C1C-NC	-3.56	1.32	1.37
31	G	610	CLA	C1C-NC	-3.56	1.32	1.37
37	B1	620	C7Z	C2-C1	3.56	1.66	1.54
31	y	604	CLA	C1C-NC	-3.56	1.32	1.37
31	G1	610	CLA	C1C-NC	-3.55	1.32	1.37
44	D	405	PL9	C3-C4	-3.55	1.43	1.49
31	c1	509	CLA	MG-ND	-3.55	1.98	2.05
31	C	506	CLA	C1C-NC	-3.55	1.32	1.37
54	i1	101	4RF	O18-C16	3.54	1.43	1.33
31	B	612	CLA	C1C-NC	-3.53	1.32	1.37
31	A1	405	CLA	C1C-NC	-3.53	1.32	1.37
31	C	504	CLA	C1C-NC	-3.53	1.32	1.37
54	I1	102	4RF	O18-C16	3.53	1.43	1.33
38	j1	101	DGA	OG2-CB1	3.53	1.44	1.34
37	B	620	C7Z	C7-C6	3.52	1.57	1.45
31	C1	502	CLA	C1C-NC	-3.52	1.32	1.37
31	C1	501	CLA	C1C-NC	-3.51	1.32	1.37
31	b	611	CLA	C1C-NC	-3.51	1.32	1.37
31	y	603	CLA	C1C-NC	-3.51	1.32	1.37
31	n	604	CLA	C1C-NC	-3.50	1.32	1.37
31	C1	504	CLA	C1C-NC	-3.50	1.32	1.37
31	b	607	CLA	C1C-NC	-3.50	1.32	1.37
37	b1	620	C7Z	C38-C25	3.50	1.56	1.50
31	C	510	CLA	C1C-NC	-3.49	1.32	1.37
31	B1	611	CLA	C1C-NC	-3.49	1.32	1.37
31	y1	610	CLA	C1C-NC	-3.48	1.32	1.37
31	C	505	CLA	C1C-NC	-3.48	1.32	1.37
37	b	620	C7Z	C38-C25	3.48	1.56	1.50
31	A	410	CLA	C1C-NC	-3.48	1.32	1.37
47	Y1	601	CHL	CBB-CAB	3.48	1.52	1.29
31	N1	604	CLA	C1C-NC	-3.48	1.32	1.37
46	h1	101	RRX	C16-C17	3.48	1.54	1.43
31	Y	602	CLA	C1C-NC	-3.47	1.32	1.37
31	C1	508	CLA	C1C-NC	-3.47	1.32	1.37
31	y	610	CLA	C1C-NC	-3.47	1.32	1.37
31	N	610	CLA	C1C-NC	-3.46	1.32	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	N1	608	CHL	CBB-CAB	3.46	1.52	1.29
31	C	502	CLA	C1C-NC	-3.46	1.32	1.37
31	C1	506	CLA	C1C-NC	-3.46	1.32	1.37
47	y1	601	CHL	CBB-CAB	3.46	1.52	1.29
31	c1	503	CLA	C1C-NC	-3.46	1.32	1.37
31	c	511	CLA	C1C-NC	-3.45	1.32	1.37
50	g1	623	NEX	C1-C6	-3.45	1.48	1.54
31	a	407	CLA	C1C-NC	-3.45	1.32	1.37
54	k1	101	4RF	O18-C16	3.45	1.43	1.33
47	Y	601	CHL	CBB-CAB	3.44	1.52	1.29
38	c1	524	DGA	OG2-CB1	3.44	1.44	1.34
31	S	612	CLA	C1C-NC	-3.44	1.32	1.37
47	s1	606	CHL	CBB-CAB	3.44	1.52	1.29
31	A	405	CLA	C1C-NC	-3.44	1.32	1.37
31	B	611	CLA	C1C-NC	-3.44	1.32	1.37
31	a	405	CLA	C1C-NC	-3.43	1.32	1.37
31	A	407	CLA	C1C-NC	-3.43	1.32	1.37
31	S1	611	CLA	C1C-NC	-3.43	1.32	1.37
47	Y1	607	CHL	CBB-CAB	3.43	1.52	1.29
47	G	609	CHL	CBB-CAB	3.42	1.52	1.29
47	N	609	CHL	CBB-CAB	3.42	1.52	1.29
47	n1	609	CHL	CBB-CAB	3.42	1.52	1.29
31	r1	604	CLA	C1C-NC	-3.42	1.32	1.37
31	C	503	CLA	C1C-NC	-3.42	1.32	1.37
31	R	612	CLA	CBB-CAB	3.42	1.52	1.29
37	B1	620	C7Z	C7-C6	3.42	1.57	1.45
31	S1	613	CLA	C1C-NC	-3.42	1.32	1.37
31	c	507	CLA	C1C-NC	-3.42	1.32	1.37
31	B1	607	CLA	C1C-NC	-3.42	1.32	1.37
31	n	604	CLA	CBB-CAB	3.42	1.52	1.29
54	K1	101	4RF	O18-C16	3.42	1.43	1.33
47	n	609	CHL	CBB-CAB	3.42	1.52	1.29
31	y1	602	CLA	CBB-CAB	3.42	1.52	1.29
31	G	603	CLA	C1C-NC	-3.42	1.32	1.37
31	a1	406	CLA	C1C-NC	-3.42	1.32	1.37
31	c	504	CLA	CBB-CAB	3.42	1.51	1.29
37	b	620	C7Z	C7-C6	3.42	1.57	1.45
37	B1	620	C7Z	C38-C25	3.41	1.56	1.50
31	g	602	CLA	CBB-CAB	3.41	1.51	1.29
31	A	406	CLA	C1C-NC	-3.41	1.32	1.37
31	B1	606	CLA	C1C-NC	-3.41	1.32	1.37
47	G	607	CHL	CBB-CAB	3.41	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	509	CLA	CBB-CAB	3.41	1.51	1.29
47	N	608	CHL	CBB-CAB	3.41	1.51	1.29
47	g1	605	CHL	CBB-CAB	3.41	1.51	1.29
31	g	604	CLA	CBB-CAB	3.41	1.51	1.29
47	g	606	CHL	CBB-CAB	3.41	1.51	1.29
38	C	524	DGA	OG2-CB1	3.41	1.43	1.34
31	C1	509	CLA	C1C-NC	-3.41	1.32	1.37
31	b1	609	CLA	CBB-CAB	3.41	1.51	1.29
47	G1	609	CHL	CBB-CAB	3.41	1.51	1.29
38	J1	101	DGA	OG2-CB1	3.41	1.43	1.34
31	c1	507	CLA	CBB-CAB	3.41	1.51	1.29
47	G	605	CHL	CBB-CAB	3.41	1.51	1.29
31	n1	602	CLA	CBB-CAB	3.40	1.51	1.29
46	H	101	RRX	C11-C10	3.40	1.54	1.43
31	S	610	CLA	C1C-NC	-3.40	1.32	1.37
31	b1	607	CLA	C1C-NC	-3.40	1.32	1.37
31	c1	509	CLA	C1C-NC	-3.40	1.32	1.37
31	b1	611	CLA	C1C-NC	-3.40	1.32	1.37
47	y	601	CHL	CBB-CAB	3.40	1.51	1.29
38	c	524	DGA	OG2-CB1	3.40	1.43	1.34
31	N1	602	CLA	CBB-CAB	3.40	1.51	1.29
47	g	601	CHL	CBB-CAB	3.40	1.51	1.29
47	y	609	CHL	CBB-CAB	3.40	1.51	1.29
31	g	603	CLA	C1C-NC	-3.40	1.32	1.37
47	Y	609	CHL	CBB-CAB	3.40	1.51	1.29
31	Y	612	CLA	C1C-NC	-3.40	1.32	1.37
31	a	410	CLA	C1C-NC	-3.40	1.32	1.37
31	C1	510	CLA	C1C-NC	-3.40	1.32	1.37
47	G1	605	CHL	CBB-CAB	3.40	1.51	1.29
31	c1	501	CLA	CBB-CAB	3.40	1.51	1.29
31	b1	608	CLA	CBB-CAB	3.39	1.51	1.29
31	Y1	603	CLA	CBB-CAB	3.39	1.51	1.29
31	n1	610	CLA	CBB-CAB	3.39	1.51	1.29
31	n	610	CLA	CBB-CAB	3.39	1.51	1.29
31	R	602	CLA	CBB-CAB	3.39	1.51	1.29
31	s1	602	CLA	CBB-CAB	3.39	1.51	1.29
47	g	608	CHL	CBB-CAB	3.39	1.51	1.29
50	Y1	623	NEX	C1-C6	-3.39	1.48	1.54
31	g	610	CLA	CBB-CAB	3.39	1.51	1.29
31	b	610	CLA	C1C-NC	-3.39	1.32	1.37
31	c1	508	CLA	CBB-CAB	3.39	1.51	1.29
47	N	607	CHL	CBB-CAB	3.39	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	610	CLA	CBB-CAB	3.39	1.51	1.29
31	B1	611	CLA	CBB-CAB	3.39	1.51	1.29
31	y	612	CLA	C1C-NC	-3.39	1.32	1.37
38	C1	524	DGA	OG2-CB1	3.39	1.43	1.34
31	n	602	CLA	CBB-CAB	3.39	1.51	1.29
31	b1	612	CLA	CBB-CAB	3.39	1.51	1.29
31	C	513	CLA	C1C-NC	-3.39	1.32	1.37
31	N	604	CLA	CBB-CAB	3.39	1.51	1.29
31	b	606	CLA	C1C-NC	-3.39	1.32	1.37
31	G	614	CLA	CBB-CAB	3.39	1.51	1.29
31	g1	602	CLA	CBB-CAB	3.39	1.51	1.29
31	n	603	CLA	CBB-CAB	3.39	1.51	1.29
31	y1	613	CLA	C1C-NC	-3.39	1.32	1.37
31	A	405	CLA	CBB-CAB	3.39	1.51	1.29
47	G1	607	CHL	CBB-CAB	3.39	1.51	1.29
31	G1	602	CLA	CBB-CAB	3.39	1.51	1.29
31	S1	612	CLA	CBB-CAB	3.39	1.51	1.29
31	n	614	CLA	CBB-CAB	3.39	1.51	1.29
47	n	605	CHL	CBB-CAB	3.39	1.51	1.29
31	B1	605	CLA	C1C-NC	-3.38	1.32	1.37
31	A1	407	CLA	CBB-CAB	3.38	1.51	1.29
31	B	615	CLA	CBB-CAB	3.38	1.51	1.29
47	S1	607	CHL	CBB-CAB	3.38	1.51	1.29
31	A1	406	CLA	CBB-CAB	3.38	1.51	1.29
47	Y	605	CHL	CBB-CAB	3.38	1.51	1.29
31	G1	603	CLA	CBB-CAB	3.38	1.51	1.29
31	A1	405	CLA	CBB-CAB	3.38	1.51	1.29
31	G	603	CLA	CBB-CAB	3.38	1.51	1.29
31	s1	613	CLA	CBB-CAB	3.38	1.51	1.29
31	C1	513	CLA	CBB-CAB	3.38	1.51	1.29
31	R1	610	CLA	CBB-CAB	3.38	1.51	1.29
47	y	607	CHL	CBB-CAB	3.38	1.51	1.29
47	G1	601	CHL	CBB-CAB	3.38	1.51	1.29
31	R1	612	CLA	CBB-CAB	3.38	1.51	1.29
31	a1	407	CLA	C1C-NC	-3.38	1.32	1.37
31	B1	612	CLA	CBB-CAB	3.38	1.51	1.29
47	n1	607	CHL	CBB-CAB	3.38	1.51	1.29
31	B1	610	CLA	CBB-CAB	3.38	1.51	1.29
31	b	613	CLA	CBB-CAB	3.38	1.51	1.29
47	N1	605	CHL	CBB-CAB	3.38	1.51	1.29
47	S1	608	CHL	CBB-CAB	3.38	1.51	1.29
47	n1	605	CHL	CBB-CAB	3.38	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n1	604	CLA	CBB-CAB	3.38	1.51	1.29
31	c	508	CLA	CBB-CAB	3.38	1.51	1.29
47	y1	609	CHL	CBB-CAB	3.38	1.51	1.29
31	a1	405	CLA	CBB-CAB	3.38	1.51	1.29
31	C	510	CLA	CBB-CAB	3.38	1.51	1.29
46	h	101	RRX	C24-C25	3.38	1.57	1.45
31	N1	614	CLA	CBB-CAB	3.38	1.51	1.29
31	b1	606	CLA	CBB-CAB	3.38	1.51	1.29
31	g	612	CLA	CBB-CAB	3.38	1.51	1.29
47	Y1	606	CHL	CBB-CAB	3.38	1.51	1.29
47	g1	607	CHL	CBB-CAB	3.37	1.51	1.29
31	S1	605	CLA	C1C-NC	-3.37	1.32	1.37
31	B1	608	CLA	CBB-CAB	3.37	1.51	1.29
31	s1	614	CLA	CBB-CAB	3.37	1.51	1.29
47	g1	601	CHL	CBB-CAB	3.37	1.51	1.29
31	R1	608	CLA	CBB-CAB	3.37	1.51	1.29
47	s1	607	CHL	CBB-CAB	3.37	1.51	1.29
31	Y1	612	CLA	CBB-CAB	3.37	1.51	1.29
47	s	607	CHL	CBB-CAB	3.37	1.51	1.29
31	G	604	CLA	C1C-NC	-3.37	1.32	1.37
47	n1	601	CHL	CBB-CAB	3.37	1.51	1.29
31	c1	511	CLA	CBB-CAB	3.37	1.51	1.29
47	y	605	CHL	CBB-CAB	3.37	1.51	1.29
31	S	617	CLA	CBB-CAB	3.37	1.51	1.29
31	r	613	CLA	CBB-CAB	3.37	1.51	1.29
31	B	608	CLA	CBB-CAB	3.37	1.51	1.29
31	b1	613	CLA	CBB-CAB	3.37	1.51	1.29
31	Y1	603	CLA	C1C-NC	-3.37	1.32	1.37
31	s	609	CLA	CBB-CAB	3.37	1.51	1.29
31	c	512	CLA	CBB-CAB	3.37	1.51	1.29
31	C1	509	CLA	CBB-CAB	3.37	1.51	1.29
31	g1	610	CLA	CBB-CAB	3.37	1.51	1.29
31	G	602	CLA	CBB-CAB	3.37	1.51	1.29
31	y	614	CLA	C1C-NC	-3.37	1.32	1.37
31	C1	508	CLA	CBB-CAB	3.37	1.51	1.29
31	B	612	CLA	CBB-CAB	3.37	1.51	1.29
31	a1	406	CLA	CBB-CAB	3.37	1.51	1.29
31	s1	604	CLA	CBB-CAB	3.37	1.51	1.29
31	s1	609	CLA	CBB-CAB	3.37	1.51	1.29
31	r	611	CLA	CBB-CAB	3.37	1.51	1.29
31	s	610	CLA	CBB-CAB	3.37	1.51	1.29
31	c1	502	CLA	CBB-CAB	3.37	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	g1	609	CHL	CBB-CAB	3.37	1.51	1.29
31	r	610	CLA	CBB-CAB	3.37	1.51	1.29
31	b	605	CLA	CBB-CAB	3.37	1.51	1.29
31	c1	512	CLA	CBB-CAB	3.37	1.51	1.29
31	N1	612	CLA	CBB-CAB	3.37	1.51	1.29
31	y1	612	CLA	CBB-CAB	3.37	1.51	1.29
31	C	507	CLA	CBB-CAB	3.37	1.51	1.29
47	n	601	CHL	CBB-CAB	3.37	1.51	1.29
47	n1	606	CHL	CBB-CAB	3.37	1.51	1.29
31	Y	608	CLA	CBB-CAB	3.37	1.51	1.29
31	g	603	CLA	CBB-CAB	3.37	1.51	1.29
31	s	604	CLA	CBB-CAB	3.37	1.51	1.29
31	B1	605	CLA	CBB-CAB	3.37	1.51	1.29
38	J1	101	DGA	OG1-CA1	3.37	1.43	1.33
31	Y1	602	CLA	CBB-CAB	3.36	1.51	1.29
47	g1	606	CHL	CBB-CAB	3.36	1.51	1.29
31	s1	605	CLA	CBB-CAB	3.36	1.51	1.29
31	N1	603	CLA	CBB-CAB	3.36	1.51	1.29
31	b1	607	CLA	CBB-CAB	3.36	1.51	1.29
37	b1	620	C7Z	C7-C6	3.36	1.57	1.45
47	Y1	605	CHL	CBB-CAB	3.36	1.51	1.29
31	r1	608	CLA	CBB-CAB	3.36	1.51	1.29
47	g	605	CHL	CBB-CAB	3.36	1.51	1.29
47	N1	601	CHL	CBB-CAB	3.36	1.51	1.29
31	R	612	CLA	C1C-NC	-3.36	1.32	1.37
31	S	605	CLA	CBB-CAB	3.36	1.51	1.29
31	G1	610	CLA	CBB-CAB	3.36	1.51	1.29
31	b1	617	CLA	CBB-CAB	3.36	1.51	1.29
31	y1	610	CLA	CBB-CAB	3.36	1.51	1.29
47	y1	605	CHL	CBB-CAB	3.36	1.51	1.29
31	B	603	CLA	CBB-CAB	3.36	1.51	1.29
31	y1	611	CLA	C1C-NC	-3.36	1.32	1.37
31	R1	609	CLA	CBB-CAB	3.36	1.51	1.29
31	S1	602	CLA	CBB-CAB	3.36	1.51	1.29
35	h1	102	LMG	C19-C18	-3.36	1.32	1.51
31	B1	606	CLA	CBB-CAB	3.36	1.51	1.29
31	n1	613	CLA	CBB-CAB	3.36	1.51	1.29
31	y1	608	CLA	CBB-CAB	3.36	1.51	1.29
31	R	604	CLA	CBB-CAB	3.36	1.51	1.29
38	c	524	DGA	OG1-CA1	3.36	1.43	1.33
31	G1	612	CLA	CBB-CAB	3.36	1.51	1.29
47	s	606	CHL	CBB-CAB	3.36	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	604	CLA	CBB-CAB	3.36	1.51	1.29
31	c1	504	CLA	CBB-CAB	3.36	1.51	1.29
31	B	602	CLA	CBB-CAB	3.36	1.51	1.29
31	y	614	CLA	CBB-CAB	3.36	1.51	1.29
31	C1	501	CLA	CBB-CAB	3.36	1.51	1.29
38	C1	524	DGA	OG1-CA1	3.36	1.43	1.33
31	S1	603	CLA	CBB-CAB	3.36	1.51	1.29
31	s1	610	CLA	CBB-CAB	3.36	1.51	1.29
31	g1	611	CLA	CBB-CAB	3.36	1.51	1.29
31	N	614	CLA	CBB-CAB	3.36	1.51	1.29
31	b	612	CLA	CBB-CAB	3.36	1.51	1.29
47	n	607	CHL	CBB-CAB	3.36	1.51	1.29
46	h	101	RRX	C11-C10	3.36	1.53	1.43
31	r	608	CLA	CBB-CAB	3.36	1.51	1.29
47	s1	601	CHL	CBB-CAB	3.36	1.51	1.29
31	b	610	CLA	CBB-CAB	3.36	1.51	1.29
31	d	403	CLA	CBB-CAB	3.36	1.51	1.29
31	g	614	CLA	CBB-CAB	3.36	1.51	1.29
31	N	602	CLA	CBB-CAB	3.36	1.51	1.29
31	n	611	CLA	CBB-CAB	3.36	1.51	1.29
31	c	507	CLA	CBB-CAB	3.36	1.51	1.29
31	G1	611	CLA	CBB-CAB	3.36	1.51	1.29
47	G	601	CHL	CBB-CAB	3.36	1.51	1.29
31	r	602	CLA	CBB-CAB	3.36	1.51	1.29
31	S1	611	CLA	CBB-CAB	3.36	1.51	1.29
31	Y	614	CLA	CBB-CAB	3.36	1.51	1.29
31	d1	402	CLA	CBB-CAB	3.36	1.51	1.29
31	C1	510	CLA	CBB-CAB	3.36	1.51	1.29
31	G	604	CLA	CBB-CAB	3.36	1.51	1.29
31	C1	512	CLA	CBB-CAB	3.36	1.51	1.29
31	S1	609	CLA	CBB-CAB	3.36	1.51	1.29
31	g1	614	CLA	CBB-CAB	3.36	1.51	1.29
31	b1	611	CLA	CBB-CAB	3.36	1.51	1.29
31	C	501	CLA	C1C-NC	-3.36	1.32	1.37
31	G	613	CLA	CBB-CAB	3.36	1.51	1.29
31	r1	602	CLA	CBB-CAB	3.36	1.51	1.29
31	b	608	CLA	CBB-CAB	3.36	1.51	1.29
31	s	603	CLA	CBB-CAB	3.36	1.51	1.29
31	s1	603	CLA	CBB-CAB	3.36	1.51	1.29
31	y1	603	CLA	CBB-CAB	3.36	1.51	1.29
31	B	614	CLA	CBB-CAB	3.36	1.51	1.29
31	S	609	CLA	CBB-CAB	3.36	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B1	616	CLA	CBB-CAB	3.36	1.51	1.29
47	r	606	CHL	CBB-CAB	3.35	1.51	1.29
47	y	606	CHL	CBB-CAB	3.35	1.51	1.29
38	C	524	DGA	OG1-CA1	3.35	1.43	1.33
31	y	610	CLA	CBB-CAB	3.35	1.51	1.29
31	D1	403	CLA	CBB-CAB	3.35	1.51	1.29
31	Y1	610	CLA	CBB-CAB	3.35	1.51	1.29
47	N	601	CHL	CBB-CAB	3.35	1.51	1.29
47	n1	608	CHL	CBB-CAB	3.35	1.51	1.29
31	B1	604	CLA	CBB-CAB	3.35	1.51	1.29
31	G	610	CLA	CBB-CAB	3.35	1.51	1.29
31	R	613	CLA	CBB-CAB	3.35	1.51	1.29
31	N	611	CLA	CBB-CAB	3.35	1.51	1.29
31	n1	611	CLA	CBB-CAB	3.35	1.51	1.29
31	g1	603	CLA	CBB-CAB	3.35	1.51	1.29
31	N1	604	CLA	CBB-CAB	3.35	1.51	1.29
31	n1	603	CLA	CBB-CAB	3.35	1.51	1.29
31	S1	610	CLA	CBB-CAB	3.35	1.51	1.29
31	N	612	CLA	CBB-CAB	3.35	1.51	1.29
47	y1	606	CHL	CBB-CAB	3.35	1.51	1.29
31	N1	610	CLA	CBB-CAB	3.35	1.51	1.29
31	c1	513	CLA	CBB-CAB	3.35	1.51	1.29
47	s1	608	CHL	CBB-CAB	3.35	1.51	1.29
31	g	613	CLA	CBB-CAB	3.35	1.51	1.29
31	C1	506	CLA	CBB-CAB	3.35	1.51	1.29
31	S	613	CLA	C1C-NC	-3.35	1.32	1.37
31	C	508	CLA	CBB-CAB	3.35	1.51	1.29
31	S1	604	CLA	CBB-CAB	3.35	1.51	1.29
31	B	610	CLA	CBB-CAB	3.35	1.51	1.29
31	c	502	CLA	CBB-CAB	3.35	1.51	1.29
47	y1	607	CHL	CBB-CAB	3.35	1.51	1.29
31	b1	605	CLA	CBB-CAB	3.35	1.51	1.29
31	g1	612	CLA	CBB-CAB	3.35	1.51	1.29
47	s	608	CHL	CBB-CAB	3.35	1.51	1.29
31	C1	507	CLA	CBB-CAB	3.35	1.51	1.29
31	b1	602	CLA	CBB-CAB	3.35	1.51	1.29
31	s1	617	CLA	CBB-CAB	3.35	1.51	1.29
31	s	611	CLA	CBB-CAB	3.35	1.51	1.29
47	G1	608	CHL	CBB-CAB	3.35	1.51	1.29
31	y1	611	CLA	CBB-CAB	3.35	1.51	1.29
31	s1	611	CLA	CBB-CAB	3.35	1.51	1.29
31	G	611	CLA	CBB-CAB	3.35	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y1	614	CLA	CBB-CAB	3.35	1.51	1.29
31	Y1	608	CLA	CBB-CAB	3.35	1.51	1.29
31	a1	410	CLA	CBB-CAB	3.35	1.51	1.29
31	s	605	CLA	CBB-CAB	3.35	1.51	1.29
31	r1	608	CLA	C1C-NC	-3.35	1.32	1.37
31	B1	609	CLA	CBB-CAB	3.35	1.51	1.29
31	r1	610	CLA	CBB-CAB	3.35	1.51	1.29
31	C	506	CLA	CBB-CAB	3.35	1.51	1.29
31	B	613	CLA	CBB-CAB	3.35	1.51	1.29
46	H	101	RRX	C16-C17	3.35	1.53	1.43
31	a	405	CLA	CBB-CAB	3.35	1.51	1.29
31	S	614	CLA	CBB-CAB	3.35	1.51	1.29
31	B1	617	CLA	CBB-CAB	3.35	1.51	1.29
47	S	608	CHL	CBB-CAB	3.35	1.51	1.29
31	B1	613	CLA	CBB-CAB	3.35	1.51	1.29
31	S1	605	CLA	CBB-CAB	3.35	1.51	1.29
31	r	604	CLA	CBB-CAB	3.35	1.51	1.29
31	b	603	CLA	CBB-CAB	3.35	1.51	1.29
31	R	611	CLA	CBB-CAB	3.35	1.51	1.29
31	G	612	CLA	CBB-CAB	3.35	1.51	1.29
47	r1	607	CHL	CBB-CAB	3.35	1.51	1.29
31	r1	603	CLA	CBB-CAB	3.35	1.51	1.29
31	S1	614	CLA	CBB-CAB	3.35	1.51	1.29
31	y	608	CLA	CBB-CAB	3.35	1.51	1.29
31	B1	602	CLA	CBB-CAB	3.35	1.51	1.29
31	R1	602	CLA	CBB-CAB	3.35	1.51	1.29
31	r1	609	CLA	CBB-CAB	3.35	1.51	1.29
47	S	606	CHL	CBB-CAB	3.35	1.51	1.29
31	N	602	CLA	C1C-NC	-3.35	1.32	1.37
31	R	603	CLA	CBB-CAB	3.35	1.51	1.29
31	s	617	CLA	CBB-CAB	3.35	1.51	1.29
31	S1	613	CLA	CBB-CAB	3.35	1.51	1.29
31	y	611	CLA	CBB-CAB	3.35	1.51	1.29
31	n1	614	CLA	CBB-CAB	3.35	1.51	1.29
31	g1	613	CLA	CBB-CAB	3.35	1.51	1.29
31	r1	604	CLA	CBB-CAB	3.35	1.51	1.29
31	r1	603	CLA	C1C-NC	-3.34	1.32	1.37
31	b	616	CLA	CBB-CAB	3.34	1.51	1.29
31	s	613	CLA	CBB-CAB	3.34	1.51	1.29
47	n	608	CHL	CBB-CAB	3.34	1.51	1.29
47	R	606	CHL	CBB-CAB	3.34	1.51	1.29
31	D1	402	CLA	CBB-CAB	3.34	1.51	1.29

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R1	604	CLA	CBB-CAB	3.34	1.51	1.29
31	Y	612	CLA	CBB-CAB	3.34	1.51	1.29
31	Y1	604	CLA	CBB-CAB	3.34	1.51	1.29
31	b	602	CLA	CBB-CAB	3.34	1.51	1.29
31	C1	504	CLA	CBB-CAB	3.34	1.51	1.29
31	Y1	611	CLA	CBB-CAB	3.34	1.51	1.29
31	B1	603	CLA	C1C-NC	-3.34	1.32	1.37
31	B1	607	CLA	CBB-CAB	3.34	1.51	1.29
31	y1	604	CLA	CBB-CAB	3.34	1.51	1.29
47	N	605	CHL	CBB-CAB	3.34	1.51	1.29
31	n1	612	CLA	CBB-CAB	3.34	1.51	1.29
31	S1	617	CLA	CBB-CAB	3.34	1.51	1.29
47	G	601	CHL	C4B-NB	3.34	1.38	1.35
31	B	614	CLA	C1C-NC	-3.34	1.32	1.37
31	n1	610	CLA	C1C-NC	-3.34	1.32	1.37
31	c	510	CLA	CBB-CAB	3.34	1.51	1.29
47	Y1	609	CHL	CBB-CAB	3.34	1.51	1.29
31	N	613	CLA	CBB-CAB	3.34	1.51	1.29
31	S	604	CLA	CBB-CAB	3.34	1.51	1.29
31	s	602	CLA	CBB-CAB	3.34	1.51	1.29
31	B	606	CLA	CBB-CAB	3.34	1.51	1.29
31	D	402	CLA	CBB-CAB	3.34	1.51	1.29
31	B	616	CLA	CBB-CAB	3.34	1.51	1.29
45	f1	101	HEM	C3C-C2C	-3.34	1.35	1.40
31	b1	603	CLA	CBB-CAB	3.34	1.51	1.29
31	Y1	613	CLA	CBB-CAB	3.34	1.51	1.29
31	b	614	CLA	CBB-CAB	3.34	1.51	1.29
31	s	614	CLA	CBB-CAB	3.34	1.51	1.29
47	G	608	CHL	CBB-CAB	3.34	1.51	1.29
31	C1	503	CLA	CBB-CAB	3.34	1.51	1.29
31	D	403	CLA	CBB-CAB	3.34	1.51	1.29
31	d	403	CLA	C1C-NC	-3.34	1.32	1.37
31	N1	611	CLA	CBB-CAB	3.34	1.51	1.29
31	R	609	CLA	CBB-CAB	3.34	1.51	1.29
31	y	613	CLA	C1C-NC	-3.34	1.32	1.37
31	y	602	CLA	CBB-CAB	3.34	1.51	1.29
31	N1	613	CLA	CBB-CAB	3.34	1.51	1.29
31	b1	604	CLA	CBB-CAB	3.34	1.51	1.29
31	s1	612	CLA	CBB-CAB	3.34	1.51	1.29
31	G	612	CLA	C1C-NC	-3.34	1.32	1.37
31	A1	407	CLA	C1C-NC	-3.34	1.32	1.37
31	C	512	CLA	CBB-CAB	3.34	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y	606	CHL	CBB-CAB	3.34	1.51	1.29
31	S	613	CLA	CBB-CAB	3.34	1.51	1.29
31	s	612	CLA	CBB-CAB	3.34	1.51	1.29
31	y1	613	CLA	CBB-CAB	3.34	1.51	1.29
31	G1	614	CLA	CBB-CAB	3.34	1.51	1.29
31	S	602	CLA	CBB-CAB	3.34	1.51	1.29
31	Y	602	CLA	CBB-CAB	3.34	1.51	1.29
31	y	613	CLA	CBB-CAB	3.34	1.51	1.29
31	b1	613	CLA	C1C-NC	-3.34	1.32	1.37
31	N	610	CLA	CBB-CAB	3.34	1.51	1.29
31	c1	505	CLA	CBB-CAB	3.34	1.51	1.29
31	G1	613	CLA	CBB-CAB	3.33	1.51	1.29
31	r	603	CLA	CBB-CAB	3.33	1.51	1.29
31	c	509	CLA	C1C-NC	-3.33	1.32	1.37
31	b1	602	CLA	C1C-NC	-3.33	1.32	1.37
31	c1	506	CLA	CBB-CAB	3.33	1.51	1.29
31	c	510	CLA	C1C-NC	-3.33	1.32	1.37
31	b1	616	CLA	CBB-CAB	3.33	1.51	1.29
31	r	609	CLA	CBB-CAB	3.33	1.51	1.29
31	b	611	CLA	CBB-CAB	3.33	1.51	1.29
31	r1	612	CLA	CBB-CAB	3.33	1.51	1.29
31	g	611	CLA	CBB-CAB	3.33	1.51	1.29
31	b1	610	CLA	CBB-CAB	3.33	1.51	1.29
31	b1	614	CLA	CBB-CAB	3.33	1.51	1.29
31	n	612	CLA	CBB-CAB	3.33	1.51	1.29
47	r1	606	CHL	CBB-CAB	3.33	1.51	1.29
31	C	512	CLA	C1C-NC	-3.33	1.32	1.37
47	s	601	CHL	C4B-NB	3.33	1.38	1.35
31	C	504	CLA	CBB-CAB	3.33	1.51	1.29
31	Y	604	CLA	CBB-CAB	3.33	1.51	1.29
31	a	407	CLA	CBB-CAB	3.33	1.51	1.29
46	h1	101	RRX	C24-C25	3.33	1.56	1.45
31	Y	614	CLA	C1C-NC	-3.33	1.32	1.37
31	N	603	CLA	CBB-CAB	3.33	1.51	1.29
31	Y	603	CLA	CBB-CAB	3.33	1.51	1.29
31	b	615	CLA	CBB-CAB	3.33	1.51	1.29
31	c	503	CLA	CBB-CAB	3.33	1.51	1.29
31	c	506	CLA	CBB-CAB	3.33	1.51	1.29
31	b	604	CLA	CBB-CAB	3.33	1.51	1.29
31	y	603	CLA	CBB-CAB	3.33	1.51	1.29
31	C	502	CLA	CBB-CAB	3.33	1.51	1.29
31	B1	604	CLA	C1C-NC	-3.33	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	612	CLA	CBB-CAB	3.33	1.51	1.29
31	y1	614	CLA	CBB-CAB	3.33	1.51	1.29
31	C	511	CLA	CBB-CAB	3.33	1.51	1.29
31	B1	603	CLA	CBB-CAB	3.33	1.51	1.29
31	G1	604	CLA	CBB-CAB	3.33	1.51	1.29
31	S1	602	CLA	C1C-NC	-3.33	1.32	1.37
47	r	607	CHL	CBB-CAB	3.33	1.51	1.29
31	C	503	CLA	CBB-CAB	3.33	1.51	1.29
31	B	609	CLA	C1C-NC	-3.33	1.32	1.37
31	S	602	CLA	C1C-NC	-3.33	1.32	1.37
38	c1	524	DGA	OG1-CA1	3.33	1.43	1.33
31	y	612	CLA	CBB-CAB	3.32	1.51	1.29
31	n	603	CLA	C1C-NC	-3.32	1.32	1.37
31	C1	505	CLA	CBB-CAB	3.32	1.51	1.29
31	A1	406	CLA	C1C-NC	-3.32	1.32	1.37
31	R	608	CLA	CBB-CAB	3.32	1.51	1.29
35	h	102	LMG	C19-C18	-3.32	1.32	1.51
31	C1	511	CLA	CBB-CAB	3.32	1.51	1.29
47	S	607	CHL	CBB-CAB	3.32	1.51	1.29
31	Y	613	CLA	CBB-CAB	3.32	1.51	1.29
31	c1	503	CLA	CBB-CAB	3.32	1.51	1.29
31	B1	614	CLA	CBB-CAB	3.32	1.51	1.29
31	n	613	CLA	CBB-CAB	3.32	1.51	1.29
47	R1	607	CHL	CBB-CAB	3.32	1.51	1.29
31	a	406	CLA	CBB-CAB	3.32	1.51	1.29
31	r	613	CLA	C1C-NC	-3.32	1.32	1.37
31	B1	610	CLA	C1C-NC	-3.32	1.32	1.37
31	y1	603	CLA	C1C-NC	-3.32	1.32	1.37
31	c	509	CLA	CBB-CAB	3.32	1.51	1.29
31	B1	615	CLA	CBB-CAB	3.32	1.51	1.29
31	Y1	604	CLA	C1C-NC	-3.32	1.32	1.37
31	Y	611	CLA	CBB-CAB	3.32	1.51	1.29
31	S	603	CLA	CBB-CAB	3.32	1.51	1.29
31	A	406	CLA	CBB-CAB	3.32	1.51	1.29
47	R1	606	CHL	CBB-CAB	3.32	1.51	1.29
31	A	407	CLA	CBB-CAB	3.32	1.51	1.29
31	B	607	CLA	CBB-CAB	3.32	1.51	1.29
31	c1	510	CLA	C1C-NC	-3.32	1.32	1.37
31	c1	501	CLA	C1C-NC	-3.32	1.32	1.37
31	g1	604	CLA	CBB-CAB	3.31	1.51	1.29
31	B	605	CLA	CBB-CAB	3.31	1.51	1.29
31	c1	510	CLA	CBB-CAB	3.31	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b1	613	CLA	C3B-C2B	-3.31	1.35	1.40
31	C	509	CLA	CBB-CAB	3.31	1.51	1.29
31	C1	502	CLA	CBB-CAB	3.31	1.51	1.29
31	r	612	CLA	CBB-CAB	3.31	1.51	1.29
31	B	616	CLA	C1C-NC	-3.31	1.32	1.37
31	Y1	613	CLA	C1C-NC	-3.31	1.32	1.37
31	C	511	CLA	C1C-NC	-3.31	1.32	1.37
31	N	612	CLA	C1C-NC	-3.31	1.32	1.37
38	j1	101	DGA	OG1-CA1	3.31	1.43	1.33
47	g	609	CHL	CBB-CAB	3.31	1.51	1.29
31	d1	403	CLA	CBB-CAB	3.31	1.51	1.29
31	c	511	CLA	CBB-CAB	3.31	1.51	1.29
47	G	606	CHL	CBB-CAB	3.31	1.51	1.29
31	C1	513	CLA	C1C-NC	-3.31	1.32	1.37
31	C	507	CLA	C1C-NC	-3.31	1.32	1.37
47	g1	608	CHL	CBB-CAB	3.31	1.51	1.29
31	g	604	CLA	C1C-NC	-3.31	1.32	1.37
38	B	625	DGA	OG1-CA1	3.31	1.43	1.33
31	C	509	CLA	C1C-NC	-3.31	1.32	1.37
31	b	607	CLA	CBB-CAB	3.31	1.51	1.29
31	d	402	CLA	CBB-CAB	3.31	1.51	1.29
47	N1	606	CHL	CBB-CAB	3.31	1.51	1.29
31	S	610	CLA	CBB-CAB	3.30	1.51	1.29
31	r1	609	CLA	C1C-NC	-3.30	1.32	1.37
38	B1	625	DGA	OG1-CA1	3.30	1.43	1.33
31	y	611	CLA	C1C-NC	-3.30	1.32	1.37
31	c1	505	CLA	C1C-NC	-3.30	1.32	1.37
31	B1	615	CLA	C1C-NC	-3.30	1.32	1.37
31	S1	612	CLA	C1C-NC	-3.30	1.32	1.37
31	a1	407	CLA	CBB-CAB	3.30	1.51	1.29
31	Y	610	CLA	CBB-CAB	3.30	1.51	1.29
31	c1	507	CLA	C1C-NC	-3.30	1.32	1.37
31	C	501	CLA	CBB-CAB	3.30	1.51	1.29
40	C	519	DGD	CDB-CCB	-3.30	1.33	1.51
31	B	611	CLA	CBB-CAB	3.30	1.51	1.29
31	C	505	CLA	CBB-CAB	3.30	1.51	1.29
31	d	402	CLA	C1C-NC	-3.30	1.32	1.37
31	b1	610	CLA	C1C-NC	-3.30	1.32	1.37
31	G1	602	CLA	C1C-NC	-3.29	1.32	1.37
46	H1	101	RRX	C11-C10	3.29	1.53	1.43
47	Y1	605	CHL	C4B-NB	3.29	1.38	1.35
31	c	512	CLA	C1C-NC	-3.29	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y1	614	CLA	C1C-NC	-3.29	1.32	1.37
31	R1	603	CLA	CBB-CAB	3.29	1.51	1.29
31	s	604	CLA	C1C-NC	-3.29	1.32	1.37
47	R	607	CHL	CBB-CAB	3.29	1.51	1.29
31	R	604	CLA	C1C-NC	-3.29	1.32	1.37
47	N1	609	CHL	CBB-CAB	3.29	1.51	1.29
31	S	614	CLA	C1C-NC	-3.29	1.32	1.37
31	G1	613	CLA	C1C-NC	-3.29	1.32	1.37
31	R1	602	CLA	C1C-NC	-3.29	1.32	1.37
31	B	615	CLA	C1C-NC	-3.29	1.32	1.37
31	S	611	CLA	CBB-CAB	3.29	1.51	1.29
31	G	602	CLA	C1C-NC	-3.29	1.32	1.37
31	Y	611	CLA	C1C-NC	-3.29	1.32	1.37
31	C	513	CLA	CBB-CAB	3.29	1.51	1.29
31	d1	402	CLA	C1C-NC	-3.29	1.32	1.37
31	B	602	CLA	C1C-NC	-3.28	1.32	1.37
31	s1	610	CLA	C1C-NC	-3.28	1.32	1.37
31	y	604	CLA	CBB-CAB	3.28	1.51	1.29
35	c1	521	LMG	C22-C21	-3.28	1.33	1.51
40	C	518	DGD	CDB-CCB	-3.28	1.33	1.51
31	b	606	CLA	CBB-CAB	3.28	1.51	1.29
47	S1	601	CHL	CBB-CAB	3.28	1.51	1.29
31	Y	604	CLA	C1C-NC	-3.28	1.32	1.37
31	Y1	612	CLA	C1C-NC	-3.28	1.32	1.37
31	c	502	CLA	C1C-NC	-3.28	1.32	1.37
40	c	523	DGD	CGA-CFA	-3.28	1.33	1.51
38	b	623	DGA	OG1-CA1	3.28	1.42	1.33
31	b	615	CLA	C1C-NC	-3.28	1.32	1.37
31	A1	410	CLA	C1C-NC	-3.28	1.32	1.37
37	B	620	C7Z	C38-C25	3.28	1.56	1.50
44	D	405	PL9	C6-C1	-3.28	1.42	1.48
40	C	520	DGD	CAB-C9B	-3.27	1.33	1.51
31	c	504	CLA	C1C-NC	-3.27	1.32	1.37
31	B1	614	CLA	C1C-NC	-3.27	1.32	1.37
47	s	606	CHL	C4B-NB	3.27	1.38	1.35
31	N	603	CLA	C1C-NC	-3.27	1.32	1.37
31	b1	615	CLA	CBB-CAB	3.27	1.51	1.29
31	Y	613	CLA	C1C-NC	-3.27	1.32	1.37
31	c	503	CLA	C1C-NC	-3.27	1.32	1.37
40	c	523	DGD	CAA-C9A	-3.27	1.33	1.51
31	b1	603	CLA	C1C-NC	-3.27	1.32	1.37
31	c1	504	CLA	C1C-NC	-3.27	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s1	611	CLA	C1C-NC	-3.27	1.32	1.37
35	H	102	LMG	C37-C36	-3.27	1.33	1.51
31	Y	603	CLA	C1C-NC	-3.27	1.32	1.37
40	C1	520	DGD	CAA-C9A	-3.27	1.33	1.51
35	C	521	LMG	C22-C21	-3.27	1.33	1.51
31	G	611	CLA	C1C-NC	-3.27	1.32	1.37
47	G1	606	CHL	CBB-CAB	3.26	1.50	1.29
35	b	622	LMG	C19-C18	-3.26	1.33	1.51
35	c	521	LMG	C40-C39	-3.26	1.33	1.51
40	c	520	DGD	CAB-C9B	-3.26	1.33	1.51
40	c	519	DGD	CDB-CCB	-3.26	1.33	1.51
47	R	606	CHL	C4B-NB	3.26	1.38	1.35
40	c	519	DGD	CAB-C9B	-3.26	1.33	1.51
31	G1	603	CLA	C1C-NC	-3.26	1.32	1.37
31	C1	511	CLA	C1C-NC	-3.26	1.32	1.37
47	s1	601	CHL	C4B-NB	3.26	1.38	1.35
47	r	606	CHL	C4B-NB	3.26	1.38	1.35
35	H	102	LMG	C19-C18	-3.26	1.33	1.51
31	g1	604	CLA	C1C-NC	-3.26	1.32	1.37
47	y1	605	CHL	C4B-NB	3.26	1.38	1.35
31	B	608	CLA	C1C-NC	-3.26	1.32	1.37
46	H	101	RRX	C24-C25	3.26	1.56	1.45
35	c1	521	LMG	C19-C18	-3.26	1.33	1.51
31	b	617	CLA	CBB-CAB	3.26	1.50	1.29
31	D	403	CLA	C1C-NC	-3.26	1.32	1.37
31	Y1	611	CLA	C1C-NC	-3.26	1.32	1.37
35	c	521	LMG	C22-C21	-3.26	1.33	1.51
31	c	513	CLA	C1C-NC	-3.26	1.32	1.37
31	C1	503	CLA	C1C-NC	-3.26	1.32	1.37
31	B	617	CLA	CBB-CAB	3.26	1.50	1.29
40	c1	518	DGD	CDB-CCB	-3.26	1.33	1.51
31	c	501	CLA	C1C-NC	-3.25	1.32	1.37
31	r	608	CLA	C1C-NC	-3.25	1.32	1.37
46	h	101	RRX	C29-C30	3.25	1.65	1.54
31	b	609	CLA	C3B-C2B	-3.25	1.35	1.40
31	S1	604	CLA	C1C-NC	-3.25	1.32	1.37
31	r1	610	CLA	C1C-NC	-3.25	1.32	1.37
31	c1	512	CLA	C1C-NC	-3.25	1.32	1.37
40	C	520	DGD	CAA-C9A	-3.25	1.33	1.51
31	r	609	CLA	C1C-NC	-3.25	1.33	1.37
31	C1	505	CLA	C1C-NC	-3.25	1.33	1.37
31	S1	609	CLA	C1C-NC	-3.25	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C1	518	DGD	CDB-CCB	-3.25	1.33	1.51
35	a	413	LMG	C37-C36	-3.25	1.33	1.51
31	b	616	CLA	C1C-NC	-3.25	1.33	1.37
35	c1	523	LMG	C37-C36	-3.25	1.33	1.51
37	B1	620	C7Z	C21-C26	-3.25	1.49	1.53
40	c	523	DGD	CAB-C9B	-3.25	1.33	1.51
31	B1	613	CLA	C1C-NC	-3.25	1.33	1.37
47	g1	608	CHL	C4B-NB	3.25	1.38	1.35
31	c	505	CLA	CBB-CAB	3.25	1.50	1.29
35	b1	622	LMG	C22-C21	-3.25	1.33	1.51
40	C1	519	DGD	CAB-C9B	-3.25	1.33	1.51
40	c	520	DGD	CAA-C9A	-3.25	1.33	1.51
47	g1	606	CHL	C4B-NB	3.25	1.38	1.35
31	B	610	CLA	C1C-NC	-3.25	1.33	1.37
31	c	505	CLA	C1C-NC	-3.25	1.33	1.37
31	s1	614	CLA	C1C-NC	-3.25	1.33	1.37
40	c1	519	DGD	CAB-C9B	-3.24	1.33	1.51
31	c	513	CLA	CBB-CAB	3.24	1.50	1.29
47	n1	605	CHL	C4B-NB	3.24	1.38	1.35
47	g1	605	CHL	C4B-NB	3.24	1.38	1.35
40	c1	519	DGD	CDA-CCA	-3.24	1.33	1.51
46	h	101	RRX	C16-C17	3.24	1.53	1.43
31	Y1	602	CLA	C1C-NC	-3.24	1.33	1.37
31	G	614	CLA	C1C-NC	-3.24	1.33	1.37
40	C	523	DGD	CDA-CCA	-3.24	1.33	1.51
31	b	614	CLA	C1C-NC	-3.24	1.33	1.37
31	S1	603	CLA	C1C-NC	-3.24	1.33	1.37
31	B	609	CLA	CBB-CAB	3.24	1.50	1.29
31	B	603	CLA	C1C-NC	-3.24	1.33	1.37
35	B1	622	LMG	C22-C21	-3.24	1.33	1.51
47	N	606	CHL	C4B-NB	3.24	1.38	1.35
31	s1	612	CLA	C1C-NC	-3.24	1.33	1.37
35	H	102	LMG	C40-C39	-3.24	1.33	1.51
31	y1	602	CLA	C1C-NC	-3.24	1.33	1.37
47	g	607	CHL	CBB-CAB	3.24	1.50	1.29
31	r	610	CLA	C1C-NC	-3.24	1.33	1.37
31	S1	614	CLA	C1C-NC	-3.24	1.33	1.37
31	g1	612	CLA	C1C-NC	-3.24	1.33	1.37
47	s1	607	CHL	C4B-NB	3.24	1.38	1.35
35	A1	413	LMG	C40-C39	-3.24	1.33	1.51
40	C1	519	DGD	CDA-CCA	-3.24	1.33	1.51
35	b	622	LMG	C22-C21	-3.23	1.33	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c1	523	LMG	C40-C39	-3.23	1.33	1.51
31	c1	508	CLA	C1C-NC	-3.23	1.33	1.37
31	n1	602	CLA	C1C-NC	-3.23	1.33	1.37
31	A1	410	CLA	CBB-CAB	3.23	1.50	1.29
31	c	501	CLA	CBB-CAB	3.23	1.50	1.29
31	b	609	CLA	CBB-CAB	3.23	1.50	1.29
35	A	413	LMG	C37-C36	-3.23	1.33	1.51
35	h	102	LMG	C37-C36	-3.23	1.33	1.51
47	S	601	CHL	C4B-NB	3.23	1.38	1.35
31	C1	507	CLA	C1C-NC	-3.23	1.33	1.37
35	C1	523	LMG	C40-C39	-3.23	1.33	1.51
40	c	519	DGD	CDA-CCA	-3.23	1.33	1.51
35	B	622	LMG	C22-C21	-3.23	1.33	1.51
35	a1	413	LMG	C37-C36	-3.23	1.33	1.51
31	R1	612	CLA	C1C-NC	-3.23	1.33	1.37
31	b	602	CLA	C1C-NC	-3.23	1.33	1.37
35	c1	523	LMG	C25-C24	-3.23	1.33	1.51
31	B1	609	CLA	C1C-NC	-3.23	1.33	1.37
31	G1	604	CLA	C1C-NC	-3.23	1.33	1.37
31	N1	612	CLA	C1C-NC	-3.23	1.33	1.37
35	C1	521	LMG	C22-C21	-3.23	1.33	1.51
31	y	602	CLA	C1C-NC	-3.23	1.33	1.37
40	C1	520	DGD	CAB-C9B	-3.23	1.33	1.51
47	n	606	CHL	C4B-NB	3.23	1.38	1.35
35	C1	523	LMG	C25-C24	-3.22	1.33	1.51
35	w1	201	LMG	C37-C36	-3.22	1.33	1.51
47	S1	601	CHL	C4B-NB	3.22	1.38	1.35
31	N1	614	CLA	C1C-NC	-3.22	1.33	1.37
35	a1	413	LMG	C40-C39	-3.22	1.33	1.51
47	r	607	CHL	C4B-NB	3.22	1.38	1.35
47	S1	608	CHL	C4B-NB	3.22	1.38	1.35
31	b	603	CLA	C1C-NC	-3.22	1.33	1.37
31	G1	611	CLA	C1C-NC	-3.22	1.33	1.37
31	s1	613	CLA	C1C-NC	-3.22	1.33	1.37
47	N1	607	CHL	CBB-CAB	3.22	1.50	1.29
35	A	413	LMG	C40-C39	-3.22	1.33	1.51
31	b	608	CLA	C1C-NC	-3.22	1.33	1.37
44	d	405	PL9	C6-C1	-3.22	1.42	1.48
35	D	411	LMG	C22-C21	-3.22	1.33	1.51
47	N	606	CHL	CBB-CAB	3.22	1.50	1.29
31	S	604	CLA	C1C-NC	-3.22	1.33	1.37
47	y1	606	CHL	C4B-NB	3.22	1.38	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G1	612	CLA	C1C-NC	-3.22	1.33	1.37
40	c	518	DGD	CDB-CCB	-3.22	1.33	1.51
35	a	413	LMG	C40-C39	-3.22	1.33	1.51
31	G1	614	CLA	C1C-NC	-3.22	1.33	1.37
47	S1	606	CHL	C4B-NB	3.22	1.38	1.35
35	h1	102	LMG	C37-C36	-3.22	1.33	1.51
31	B	606	CLA	C1C-NC	-3.22	1.33	1.37
31	B1	612	CLA	C1C-NC	-3.22	1.33	1.37
40	C	523	DGD	CGA-CFA	-3.22	1.33	1.51
46	H1	101	RRX	C16-C17	3.21	1.53	1.43
31	N	613	CLA	C1C-NC	-3.21	1.33	1.37
35	W1	201	LMG	C40-C39	-3.21	1.33	1.51
35	C1	523	LMG	C37-C36	-3.21	1.33	1.51
35	W1	201	LMG	C37-C36	-3.21	1.33	1.51
31	B	613	CLA	C1C-NC	-3.21	1.33	1.37
31	s	610	CLA	C1C-NC	-3.21	1.33	1.37
35	H1	102	LMG	C19-C18	-3.21	1.33	1.51
31	B1	608	CLA	C1C-NC	-3.21	1.33	1.37
35	B	622	LMG	C19-C18	-3.21	1.33	1.51
31	a1	405	CLA	C1C-NC	-3.21	1.33	1.37
47	R1	606	CHL	C4B-NB	3.21	1.38	1.35
31	b	604	CLA	C1C-NC	-3.21	1.33	1.37
40	c1	518	DGD	CAB-C9B	-3.21	1.33	1.51
35	B1	622	LMG	C19-C18	-3.21	1.33	1.51
31	N1	613	CLA	C1C-NC	-3.21	1.33	1.37
35	J	101	LMG	C22-C21	-3.21	1.33	1.51
35	d1	411	LMG	C19-C18	-3.21	1.33	1.51
40	C1	518	DGD	CAB-C9B	-3.21	1.33	1.51
31	B	604	CLA	C1C-NC	-3.21	1.33	1.37
35	C1	523	LMG	C43-C42	-3.21	1.33	1.51
35	A1	413	LMG	C37-C36	-3.21	1.33	1.51
31	S1	617	CLA	C1C-NC	-3.21	1.33	1.37
31	b1	606	CLA	C1C-NC	-3.21	1.33	1.37
31	s	609	CLA	C1C-NC	-3.21	1.33	1.37
31	B	605	CLA	C3B-C2B	-3.21	1.35	1.40
31	n	613	CLA	C1C-NC	-3.21	1.33	1.37
31	s1	602	CLA	C1C-NC	-3.21	1.33	1.37
35	a	413	LMG	C19-C18	-3.21	1.33	1.51
47	G	606	CHL	C4B-NB	3.21	1.38	1.35
35	C1	521	LMG	C40-C39	-3.20	1.33	1.51
35	c1	523	LMG	C22-C21	-3.20	1.33	1.51
31	g1	610	CLA	C1C-NC	-3.20	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	519	DGD	CAB-C9B	-3.20	1.33	1.51
31	S	605	CLA	C1C-NC	-3.20	1.33	1.37
40	C	523	DGD	CAA-C9A	-3.20	1.33	1.51
31	n	612	CLA	C1C-NC	-3.20	1.33	1.37
31	d1	403	CLA	C1C-NC	-3.20	1.33	1.37
35	C	521	LMG	C19-C18	-3.20	1.33	1.51
40	C	519	DGD	CDA-CCA	-3.20	1.33	1.51
31	g	612	CLA	C1C-NC	-3.20	1.33	1.37
31	s	603	CLA	C1C-NC	-3.20	1.33	1.37
31	R1	604	CLA	C1C-NC	-3.20	1.33	1.37
35	H1	102	LMG	C37-C36	-3.20	1.33	1.51
31	n1	612	CLA	C1C-NC	-3.20	1.33	1.37
40	c	523	DGD	CDA-CCA	-3.20	1.33	1.51
40	c	523	DGD	CGB-CFB	-3.20	1.33	1.51
35	C1	523	LMG	C22-C21	-3.20	1.33	1.51
35	d	411	LMG	C22-C21	-3.20	1.33	1.51
35	H1	102	LMG	C40-C39	-3.20	1.33	1.51
31	A	410	CLA	CBB-CAB	3.20	1.50	1.29
31	n	611	CLA	C1C-NC	-3.20	1.33	1.37
40	C1	519	DGD	CDB-CCB	-3.20	1.33	1.51
47	s1	608	CHL	C4B-NB	3.19	1.38	1.35
31	y1	614	CLA	C1C-NC	-3.19	1.33	1.37
46	H1	101	RRX	C24-C25	3.19	1.56	1.45
35	C1	521	LMG	C19-C18	-3.19	1.33	1.51
47	Y	607	CHL	CBB-CAB	3.19	1.50	1.29
31	R	608	CLA	C1C-NC	-3.19	1.33	1.37
31	g	610	CLA	C1C-NC	-3.19	1.33	1.37
31	N1	603	CLA	C1C-NC	-3.19	1.33	1.37
31	s1	604	CLA	C1C-NC	-3.19	1.33	1.37
31	g	611	CLA	C1C-NC	-3.19	1.33	1.37
35	D1	411	LMG	C19-C18	-3.19	1.33	1.51
47	n1	601	CHL	C4B-NB	3.19	1.38	1.35
47	s	601	CHL	CBB-CAB	3.19	1.50	1.29
35	c1	523	LMG	C43-C42	-3.19	1.33	1.51
40	c	523	DGD	CDB-CCB	-3.19	1.33	1.51
31	b1	604	CLA	C1C-NC	-3.19	1.33	1.37
47	S	608	CHL	C4B-NB	3.19	1.38	1.35
31	N	611	CLA	C1C-NC	-3.19	1.33	1.37
31	r	604	CLA	C1C-NC	-3.19	1.33	1.37
40	C	520	DGD	CDB-CCB	-3.19	1.33	1.51
40	c	518	DGD	CAB-C9B	-3.19	1.33	1.51
35	J	101	LMG	C19-C18	-3.19	1.33	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	518	DGD	CAB-C9B	-3.19	1.33	1.51
35	C	521	LMG	C40-C39	-3.19	1.33	1.51
35	d1	411	LMG	C22-C21	-3.19	1.33	1.51
47	S	601	CHL	CBB-CAB	3.19	1.50	1.29
31	N1	602	CLA	C1C-NC	-3.19	1.33	1.37
47	y	606	CHL	C4B-NB	3.19	1.38	1.35
31	a	410	CLA	CBB-CAB	3.19	1.50	1.29
47	n	601	CHL	C4B-NB	3.19	1.38	1.35
35	b1	622	LMG	C19-C18	-3.19	1.33	1.51
31	s1	605	CLA	C1C-NC	-3.19	1.33	1.37
35	a1	413	LMG	C19-C18	-3.19	1.33	1.51
46	H1	101	RRX	C29-C30	3.19	1.64	1.54
31	N	614	CLA	C1C-NC	-3.19	1.33	1.37
35	h	102	LMG	C40-C39	-3.19	1.33	1.51
35	c	521	LMG	C37-C36	-3.18	1.33	1.51
35	c	521	LMG	C19-C18	-3.18	1.33	1.51
31	r1	602	CLA	C1C-NC	-3.18	1.33	1.37
40	c1	520	DGD	CDB-CCB	-3.18	1.33	1.51
35	A	413	LMG	C19-C18	-3.18	1.33	1.51
40	c1	520	DGD	CAA-C9A	-3.18	1.33	1.51
35	c1	521	LMG	C40-C39	-3.18	1.33	1.51
31	R1	603	CLA	C1C-NC	-3.18	1.33	1.37
45	F1	101	HEM	CAB-C3B	3.18	1.56	1.47
35	j	101	LMG	C19-C18	-3.18	1.33	1.51
31	R1	609	CLA	C1C-NC	-3.18	1.33	1.37
40	c1	519	DGD	CAA-C9A	-3.18	1.33	1.51
40	C1	519	DGD	CAA-C9A	-3.18	1.33	1.51
35	D1	411	LMG	C22-C21	-3.18	1.33	1.51
35	C	521	LMG	C37-C36	-3.18	1.33	1.51
31	R	611	CLA	C1C-NC	-3.18	1.33	1.37
40	C	523	DGD	CAB-C9B	-3.18	1.33	1.51
47	g1	601	CHL	C4B-NB	3.18	1.38	1.35
40	C	523	DGD	CDB-CCB	-3.18	1.33	1.51
31	g	614	CLA	C1C-NC	-3.18	1.33	1.37
45	f1	101	HEM	CAB-C3B	3.18	1.56	1.47
31	s1	603	CLA	C1C-NC	-3.18	1.33	1.37
47	g	609	CHL	C4B-NB	3.18	1.38	1.35
47	Y1	606	CHL	C4B-NB	3.17	1.38	1.35
35	A1	413	LMG	C19-C18	-3.17	1.33	1.51
47	n1	606	CHL	C4B-NB	3.17	1.38	1.35
31	n1	603	CLA	C1C-NC	-3.17	1.33	1.37
40	c1	520	DGD	CAB-C9B	-3.17	1.33	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S1	607	CHL	C4B-NB	3.17	1.38	1.35
31	y1	604	CLA	C1C-NC	-3.17	1.33	1.37
40	C	523	DGD	CGB-CFB	-3.17	1.33	1.51
35	j	101	LMG	C22-C21	-3.17	1.33	1.51
35	c1	523	LMG	C19-C18	-3.17	1.33	1.51
31	c1	511	CLA	C1C-NC	-3.17	1.33	1.37
47	g	601	CHL	C4B-NB	3.17	1.38	1.35
47	y1	609	CHL	C4B-NB	3.17	1.38	1.35
31	g1	613	CLA	C1C-NC	-3.17	1.33	1.37
38	b1	625	DGA	OG1-CA1	3.17	1.42	1.33
35	h1	102	LMG	C40-C39	-3.17	1.33	1.51
47	Y1	609	CHL	C4B-NB	3.17	1.38	1.35
35	C1	523	LMG	C19-C18	-3.17	1.33	1.51
47	S1	606	CHL	CBB-CAB	3.17	1.50	1.29
31	n1	604	CLA	C1C-NC	-3.16	1.33	1.37
31	n1	614	CLA	C1C-NC	-3.16	1.33	1.37
35	D	411	LMG	C19-C18	-3.16	1.33	1.51
31	s	613	CLA	C1C-NC	-3.16	1.33	1.37
40	c	520	DGD	CDB-CCB	-3.16	1.33	1.51
31	N1	611	CLA	C1C-NC	-3.16	1.33	1.37
31	b1	616	CLA	C1C-NC	-3.16	1.33	1.37
40	c	519	DGD	CAA-C9A	-3.16	1.33	1.51
47	G1	606	CHL	C4B-NB	3.16	1.38	1.35
47	G	605	CHL	C4B-NB	3.16	1.38	1.35
47	s	607	CHL	C4B-NB	3.16	1.38	1.35
31	b1	605	CLA	C3B-C2B	-3.16	1.36	1.40
31	c1	513	CLA	C1C-NC	-3.16	1.33	1.37
40	C1	520	DGD	CDB-CCB	-3.16	1.33	1.51
35	c1	521	LMG	C37-C36	-3.15	1.33	1.51
31	D1	403	CLA	C1C-NC	-3.15	1.33	1.37
31	b1	615	CLA	C1C-NC	-3.15	1.33	1.37
47	y	605	CHL	C4B-NB	3.15	1.38	1.35
46	h1	101	RRX	C29-C30	3.15	1.64	1.54
31	g1	614	CLA	C1C-NC	-3.15	1.33	1.37
40	c1	519	DGD	CDB-CCB	-3.15	1.33	1.51
47	G	608	CHL	C4B-NB	3.15	1.38	1.35
31	s	612	CLA	C1C-NC	-3.15	1.33	1.37
47	S	606	CHL	C4B-NB	3.15	1.38	1.35
47	s	608	CHL	C4B-NB	3.15	1.38	1.35
40	C	519	DGD	CAA-C9A	-3.15	1.33	1.51
47	g	608	CHL	C4B-NB	3.15	1.38	1.35
31	S	609	CLA	C1C-NC	-3.15	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y1	608	CLA	C1C-NC	-3.14	1.33	1.37
31	R	610	CLA	C1C-NC	-3.14	1.33	1.37
31	N	604	CLA	C1C-NC	-3.14	1.33	1.37
31	b1	614	CLA	C1C-NC	-3.14	1.33	1.37
35	w1	201	LMG	C40-C39	-3.14	1.33	1.51
47	N	601	CHL	C4B-NB	3.14	1.38	1.35
35	C1	521	LMG	C37-C36	-3.14	1.33	1.51
31	B1	602	CLA	C1C-NC	-3.14	1.33	1.37
31	S	603	CLA	C1C-NC	-3.14	1.33	1.37
47	r1	607	CHL	C4B-NB	3.14	1.38	1.35
31	S	611	CLA	C1C-NC	-3.14	1.33	1.37
35	d	411	LMG	C19-C18	-3.14	1.34	1.51
47	N1	605	CHL	C4B-NB	3.14	1.38	1.35
47	g1	609	CHL	C4B-NB	3.14	1.38	1.35
54	k1	101	4RF	O40-C41	3.14	1.42	1.33
47	g	605	CHL	C4B-NB	3.14	1.38	1.35
31	R	613	CLA	C1C-NC	-3.13	1.33	1.37
47	N1	606	CHL	C4B-NB	3.13	1.38	1.35
47	G1	605	CHL	C4B-NB	3.13	1.38	1.35
47	n	606	CHL	CBB-CAB	3.13	1.50	1.29
47	R1	607	CHL	C4B-NB	3.13	1.38	1.35
31	s	614	CLA	C1C-NC	-3.13	1.33	1.37
47	Y	605	CHL	C4B-NB	3.13	1.38	1.35
47	R	607	CHL	C4B-NB	3.13	1.38	1.35
47	Y	606	CHL	C4B-NB	3.12	1.38	1.35
31	g1	603	CLA	C1C-NC	-3.12	1.33	1.37
47	Y	609	CHL	C4B-NB	3.12	1.38	1.35
31	B	607	CLA	C1C-NC	-3.12	1.33	1.37
31	g1	602	CLA	C1C-NC	-3.12	1.33	1.37
31	r	603	CLA	C1C-NC	-3.12	1.33	1.37
31	r	602	CLA	C1C-NC	-3.12	1.33	1.37
31	n1	611	CLA	C1C-NC	-3.12	1.33	1.37
46	H	101	RRX	C29-C30	3.12	1.64	1.54
31	R1	608	CLA	C1C-NC	-3.11	1.33	1.37
31	c1	506	CLA	C1C-NC	-3.11	1.33	1.37
31	R	602	CLA	C1C-NC	-3.11	1.33	1.37
31	a1	410	CLA	C1C-NC	-3.10	1.33	1.37
31	y	608	CLA	C1C-NC	-3.10	1.33	1.37
47	y	609	CHL	C4B-NB	3.10	1.38	1.35
31	C1	512	CLA	C1C-NC	-3.10	1.33	1.37
31	s1	617	CLA	C1C-NC	-3.10	1.33	1.37
31	n	602	CLA	C1C-NC	-3.09	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	r1	606	CHL	C4B-NB	3.09	1.38	1.35
47	n	605	CHL	C4B-NB	3.09	1.38	1.35
31	s1	609	CLA	C1C-NC	-3.09	1.33	1.37
46	h	101	RRX	C4-C5	-3.09	1.44	1.51
31	S	617	CLA	C1C-NC	-3.09	1.33	1.37
31	g	613	CLA	C1C-NC	-3.09	1.33	1.37
31	G	613	CLA	C1C-NC	-3.09	1.33	1.37
31	R1	610	CLA	C1C-NC	-3.09	1.33	1.37
31	y1	608	CLA	C1C-NC	-3.09	1.33	1.37
31	b1	608	CLA	C1C-NC	-3.08	1.33	1.37
31	n1	613	CLA	C1C-NC	-3.08	1.33	1.37
31	b	609	CLA	C1C-NC	-3.08	1.33	1.37
47	S	607	CHL	C4B-NB	3.08	1.38	1.35
47	G1	608	CHL	C4B-NB	3.08	1.38	1.35
44	D1	405	PL9	C6-C1	-3.08	1.43	1.48
31	n	614	CLA	C1C-NC	-3.08	1.33	1.37
47	N	605	CHL	C4B-NB	3.08	1.38	1.35
31	r1	612	CLA	C1C-NC	-3.07	1.33	1.37
31	s	611	CLA	C1C-NC	-3.07	1.33	1.37
31	R	603	CLA	C1C-NC	-3.07	1.33	1.37
31	s	605	CLA	C1C-NC	-3.07	1.33	1.37
46	h1	101	RRX	C7-C6	3.07	1.56	1.45
47	N	608	CHL	C4B-NB	3.07	1.37	1.35
54	I1	102	4RF	O40-C41	3.06	1.42	1.33
31	r	611	CLA	C1C-NC	-3.06	1.33	1.37
47	N1	601	CHL	C4B-NB	3.06	1.37	1.35
31	C1	502	CLA	C3B-C2B	-3.05	1.36	1.40
31	R	609	CLA	C1C-NC	-3.04	1.33	1.37
31	g1	611	CLA	C1C-NC	-3.04	1.33	1.37
45	f	101	HEM	CAB-C3B	3.03	1.55	1.47
54	K1	101	4RF	O40-C41	3.03	1.42	1.33
31	r	612	CLA	C1C-NC	-3.03	1.33	1.37
31	B1	612	CLA	CHC-C1C	3.03	1.42	1.35
47	n1	608	CHL	C4B-NB	3.03	1.37	1.35
31	Y	608	CLA	C1C-NC	-3.02	1.33	1.37
31	y1	612	CLA	C1C-NC	-3.02	1.33	1.37
31	S	611	CLA	C3B-C2B	-3.01	1.36	1.40
54	i1	101	4RF	O40-C41	3.01	1.42	1.33
47	g1	607	CHL	C4B-NB	3.01	1.37	1.35
46	H	101	RRX	C4-C5	-3.00	1.45	1.51
47	n	608	CHL	C4B-NB	3.00	1.37	1.35
46	h	101	RRX	C7-C6	3.00	1.55	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	y1	607	CHL	C4B-NB	3.00	1.37	1.35
47	n	607	CHL	C4B-NB	2.99	1.37	1.35
31	s	617	CLA	C1C-NC	-2.97	1.33	1.37
46	H1	101	RRX	C4-C5	-2.97	1.45	1.51
31	g	602	CLA	C1C-NC	-2.95	1.33	1.37
51	S1	625	LPX	P1-O1	2.94	1.71	1.59
46	H1	101	RRX	C7-C6	2.94	1.55	1.45
46	H	101	RRX	C7-C6	2.94	1.55	1.45
46	h1	101	RRX	C4-C5	-2.93	1.45	1.51
47	N	606	CHL	C3B-C2B	-2.93	1.36	1.40
51	S	625	LPX	P1-O1	2.92	1.71	1.59
51	s1	625	LPX	P1-O1	2.91	1.71	1.59
31	b1	609	CLA	C1C-NC	-2.91	1.33	1.37
47	G1	601	CHL	C4B-NB	2.91	1.37	1.35
51	s	625	LPX	P1-O1	2.91	1.71	1.59
47	s1	606	CHL	C4B-NB	2.90	1.37	1.35
31	d	402	CLA	CHC-C1C	2.90	1.42	1.35
47	G1	609	CHL	C4B-NB	2.90	1.37	1.35
47	y	607	CHL	C4B-NB	2.90	1.37	1.35
47	n1	609	CHL	C4B-NB	2.90	1.37	1.35
31	c1	508	CLA	CHC-C1C	2.89	1.42	1.35
47	y1	601	CHL	C4B-NB	2.88	1.37	1.35
31	y1	602	CLA	CHC-C1C	2.87	1.42	1.35
31	c1	505	CLA	C3B-C2B	-2.87	1.36	1.40
47	Y1	601	CHL	C4B-NB	2.87	1.37	1.35
54	I1	102	4RF	O21-C22	2.87	1.42	1.34
56	R1	626	ERG	C9-C8	2.86	1.59	1.51
31	s1	602	CLA	CHC-C1C	2.86	1.42	1.35
31	B	612	CLA	CHC-C1C	2.86	1.42	1.35
31	A1	405	CLA	CHC-C1C	2.86	1.42	1.35
46	h1	101	RRX	C32-C1	2.86	1.59	1.53
31	N	610	CLA	CHC-C1C	2.85	1.42	1.35
47	G	607	CHL	C4B-NB	2.85	1.37	1.35
47	G	609	CHL	C4B-NB	2.85	1.37	1.35
47	Y	601	CHL	C4B-NB	2.84	1.37	1.35
56	R1	626	ERG	C4-C5	2.84	1.57	1.51
32	a	408	PHO	CAC-C3C	-2.84	1.47	1.52
47	g	606	CHL	C4B-NB	2.83	1.37	1.35
31	n	612	CLA	CHC-C1C	2.83	1.42	1.35
47	N1	608	CHL	C4B-NB	2.83	1.37	1.35
45	F	101	HEM	CAB-C3B	2.83	1.55	1.47
31	R1	610	CLA	CHC-C1C	2.82	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	604	CLA	CHC-C1C	2.82	1.42	1.35
31	g1	602	CLA	CHC-C1C	2.82	1.42	1.35
31	y	602	CLA	CHC-C1C	2.81	1.42	1.35
31	b	612	CLA	CHC-C1C	2.80	1.42	1.35
47	n	609	CHL	C4B-NB	2.80	1.37	1.35
31	r	610	CLA	CHC-C1C	2.80	1.42	1.35
47	S1	606	CHL	C3B-C2B	-2.80	1.36	1.40
47	N1	607	CHL	C4B-NB	2.80	1.37	1.35
31	s	612	CLA	CHC-C1C	2.79	1.42	1.35
31	c	511	CLA	CHC-C1C	2.79	1.42	1.35
31	r1	602	CLA	CHC-C1C	2.78	1.42	1.35
32	A	409	PHO	CAC-C3C	-2.78	1.47	1.52
31	G1	602	CLA	CHC-C1C	2.78	1.42	1.35
56	r1	626	ERG	C4-C5	2.78	1.57	1.51
31	n	614	CLA	CHC-C1C	2.78	1.42	1.35
50	r1	622	NEX	C1-C6	-2.78	1.49	1.54
31	c1	513	CLA	CHC-C1C	2.78	1.42	1.35
31	Y	602	CLA	CHC-C1C	2.77	1.42	1.35
31	B	606	CLA	CHC-C1C	2.77	1.42	1.35
54	i1	101	4RF	O21-C22	2.77	1.42	1.34
47	Y	607	CHL	C4B-NB	2.76	1.37	1.35
47	N	609	CHL	C4B-NB	2.76	1.37	1.35
31	R	609	CLA	CHC-C1C	2.76	1.42	1.35
31	g	610	CLA	CHC-C1C	2.76	1.42	1.35
31	A1	406	CLA	CHC-C1C	2.76	1.42	1.35
31	R	602	CLA	CHC-C1C	2.76	1.42	1.35
31	n	604	CLA	CHC-C1C	2.76	1.42	1.35
31	c1	507	CLA	CHC-C1C	2.76	1.42	1.35
47	y	601	CHL	C4B-NB	2.76	1.37	1.35
46	H	101	RRX	C32-C1	2.75	1.59	1.53
31	r	602	CLA	CHC-C1C	2.75	1.42	1.35
47	n1	607	CHL	C4B-NB	2.75	1.37	1.35
47	g	607	CHL	C4B-NB	2.75	1.37	1.35
31	c1	511	CLA	CHC-C1C	2.75	1.42	1.35
54	k1	101	4RF	O21-C22	2.75	1.42	1.34
31	G	603	CLA	C3B-C2B	-2.75	1.36	1.40
47	Y1	607	CHL	C4B-NB	2.74	1.37	1.35
31	n1	614	CLA	CHC-C1C	2.74	1.42	1.35
31	s	609	CLA	CHC-C1C	2.74	1.42	1.35
31	N1	602	CLA	CHC-C1C	2.74	1.42	1.35
50	R	622	NEX	C1-C6	-2.74	1.50	1.54
31	r	612	CLA	CHC-C1C	2.73	1.42	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	610	CLA	CHC-C1C	2.73	1.42	1.35
31	B1	604	CLA	CHC-C1C	2.73	1.42	1.35
31	R	609	CLA	C3B-C2B	-2.73	1.36	1.40
31	Y1	602	CLA	CHC-C1C	2.73	1.42	1.35
31	B	604	CLA	CHC-C1C	2.73	1.42	1.35
31	G	610	CLA	CHC-C1C	2.73	1.42	1.35
31	B	602	CLA	C3B-C2B	-2.73	1.36	1.40
31	C1	513	CLA	CHC-C1C	2.72	1.41	1.35
31	a1	410	CLA	CHC-C1C	2.72	1.41	1.35
31	B1	610	CLA	CHC-C1C	2.72	1.41	1.35
31	R1	603	CLA	C3B-C2B	-2.72	1.36	1.40
46	h	101	RRX	C32-C1	2.72	1.59	1.53
31	S	617	CLA	CHC-C1C	2.72	1.41	1.35
31	N	613	CLA	CHC-C1C	2.72	1.41	1.35
31	g1	610	CLA	CHC-C1C	2.72	1.41	1.35
31	n	602	CLA	CHC-C1C	2.71	1.41	1.35
32	a1	408	PHO	CAC-C3C	-2.71	1.47	1.52
31	S	609	CLA	CHC-C1C	2.71	1.41	1.35
31	D1	402	CLA	C3B-C2B	-2.71	1.36	1.40
31	r	611	CLA	CHC-C1C	2.71	1.41	1.35
31	B	617	CLA	C3B-C2B	-2.71	1.36	1.40
31	g	614	CLA	CHC-C1C	2.70	1.41	1.35
54	K1	101	4RF	O21-C22	2.70	1.41	1.34
31	n	611	CLA	CHC-C1C	2.70	1.41	1.35
31	C1	504	CLA	C3B-C2B	-2.70	1.36	1.40
31	C1	508	CLA	CHC-C1C	2.70	1.41	1.35
47	n	606	CHL	C3B-C2B	-2.70	1.36	1.40
31	b	607	CLA	C3B-C2B	-2.69	1.36	1.40
31	c	501	CLA	CHC-C1C	2.69	1.41	1.35
31	c	513	CLA	CHC-C1C	2.69	1.41	1.35
50	s1	623	NEX	C1-C6	-2.69	1.50	1.54
31	s	614	CLA	C3B-C2B	-2.69	1.36	1.40
31	R	611	CLA	CHC-C1C	2.68	1.41	1.35
31	y	603	CLA	C3B-C2B	-2.68	1.36	1.40
31	g1	614	CLA	CHC-C1C	2.68	1.41	1.35
47	N	607	CHL	C4B-NB	2.68	1.37	1.35
31	Y	608	CLA	CHC-C1C	2.68	1.41	1.35
31	G1	612	CLA	C3B-C2B	-2.68	1.36	1.40
31	y1	603	CLA	C3B-C2B	-2.68	1.36	1.40
31	C1	512	CLA	CHC-C1C	2.68	1.41	1.35
31	B	611	CLA	CHC-C1C	2.67	1.41	1.35
31	G	614	CLA	CHC-C1C	2.67	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	N1	609	CHL	C4B-NB	2.67	1.37	1.35
31	c	503	CLA	C3B-C2B	-2.67	1.36	1.40
31	R	613	CLA	CHC-C1C	2.67	1.41	1.35
31	n1	612	CLA	CHC-C1C	2.67	1.41	1.35
31	n1	611	CLA	CHC-C1C	2.67	1.41	1.35
31	r1	610	CLA	CHC-C1C	2.67	1.41	1.35
31	G	613	CLA	CHC-C1C	2.67	1.41	1.35
31	d1	402	CLA	C3B-C2B	-2.67	1.36	1.40
31	Y	604	CLA	CHC-C1C	2.67	1.41	1.35
31	S	613	CLA	C3B-C2B	-2.67	1.36	1.40
56	r1	626	ERG	C9-C8	2.67	1.58	1.51
31	n1	613	CLA	CHC-C1C	2.67	1.41	1.35
31	A1	407	CLA	CHC-C1C	2.67	1.41	1.35
31	G1	610	CLA	CHC-C1C	2.67	1.41	1.35
55	R1	625	LMT	O3'-C3'	-2.67	1.36	1.43
31	r	612	CLA	C3B-C2B	-2.66	1.36	1.40
31	R	608	CLA	C3B-C2B	-2.66	1.36	1.40
31	D	402	CLA	CHC-C1C	2.66	1.41	1.35
31	N	603	CLA	C3B-C2B	-2.66	1.36	1.40
31	B	603	CLA	C3B-C2B	-2.66	1.36	1.40
31	c	510	CLA	CHC-C1C	2.66	1.41	1.35
31	g1	604	CLA	CHC-C1C	2.66	1.41	1.35
31	C	503	CLA	CHC-C1C	2.66	1.41	1.35
31	R	603	CLA	CHC-C1C	2.66	1.41	1.35
31	b	606	CLA	C3B-C2B	-2.66	1.36	1.40
31	D	403	CLA	CHC-C1C	2.66	1.41	1.35
31	d1	403	CLA	CHC-C1C	2.66	1.41	1.35
31	s1	610	CLA	C3B-C2B	-2.66	1.36	1.40
31	N1	610	CLA	C3B-C2B	-2.65	1.36	1.40
31	B	608	CLA	CHC-C1C	2.65	1.41	1.35
31	G	611	CLA	CHC-C1C	2.65	1.41	1.35
31	D1	402	CLA	CHC-C1C	2.65	1.41	1.35
31	g	612	CLA	CHC-C1C	2.65	1.41	1.35
31	g	612	CLA	C3B-C2B	-2.65	1.36	1.40
31	c1	503	CLA	C3B-C2B	-2.65	1.36	1.40
31	n	613	CLA	CHC-C1C	2.65	1.41	1.35
31	s	617	CLA	CHC-C1C	2.65	1.41	1.35
31	y1	604	CLA	CHC-C1C	2.65	1.41	1.35
47	G1	607	CHL	C4B-NB	2.65	1.37	1.35
31	N1	614	CLA	CHC-C1C	2.65	1.41	1.35
31	R1	604	CLA	C3B-C2B	-2.65	1.36	1.40
47	G	606	CHL	C3B-C2B	-2.65	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	602	CLA	CHC-C1C	2.65	1.41	1.35
31	s	610	CLA	CHC-C1C	2.65	1.41	1.35
31	c	505	CLA	C3B-C2B	-2.65	1.36	1.40
31	R	610	CLA	CHC-C1C	2.65	1.41	1.35
31	D1	403	CLA	CHC-C1C	2.64	1.41	1.35
31	s	611	CLA	C3B-C2B	-2.64	1.36	1.40
31	Y	613	CLA	CHC-C1C	2.64	1.41	1.35
31	b1	616	CLA	C3B-C2B	-2.64	1.36	1.40
31	N	602	CLA	CHC-C1C	2.64	1.41	1.35
31	g	604	CLA	CHC-C1C	2.64	1.41	1.35
31	n1	610	CLA	CHC-C1C	2.64	1.41	1.35
46	H1	101	RRX	C32-C1	2.64	1.59	1.53
31	r	604	CLA	CHC-C1C	2.64	1.41	1.35
31	Y	610	CLA	CHC-C1C	2.64	1.41	1.35
31	b1	606	CLA	CHC-C1C	2.64	1.41	1.35
31	y	608	CLA	CHC-C1C	2.64	1.41	1.35
31	G1	612	CLA	CHC-C1C	2.64	1.41	1.35
31	N	611	CLA	CHC-C1C	2.64	1.41	1.35
31	b	602	CLA	C3B-C2B	-2.64	1.36	1.40
47	G	601	CHL	C3A-C2A	-2.64	1.47	1.54
31	g1	613	CLA	CHC-C1C	2.64	1.41	1.35
31	g1	611	CLA	CHC-C1C	2.64	1.41	1.35
31	C1	506	CLA	C3B-C2B	-2.64	1.36	1.40
31	g	602	CLA	CHC-C1C	2.64	1.41	1.35
31	g	611	CLA	CHC-C1C	2.64	1.41	1.35
31	R1	602	CLA	CHC-C1C	2.64	1.41	1.35
31	B1	607	CLA	CHC-C1C	2.63	1.41	1.35
31	S	610	CLA	C3B-C2B	-2.63	1.36	1.40
31	c	501	CLA	C3B-C2B	-2.63	1.36	1.40
31	s	603	CLA	CHC-C1C	2.63	1.41	1.35
31	y	604	CLA	C3B-C2B	-2.63	1.36	1.40
31	b1	608	CLA	CHC-C1C	2.63	1.41	1.35
31	y1	608	CLA	CHC-C1C	2.63	1.41	1.35
31	y1	612	CLA	CHC-C1C	2.63	1.41	1.35
31	S1	609	CLA	CHC-C1C	2.62	1.41	1.35
31	Y1	614	CLA	CHC-C1C	2.62	1.41	1.35
31	C	505	CLA	C3B-C2B	-2.62	1.36	1.40
31	c1	512	CLA	CHC-C1C	2.62	1.41	1.35
31	A	407	CLA	C3B-C2B	-2.62	1.36	1.40
31	r	609	CLA	CHC-C1C	2.62	1.41	1.35
31	c1	505	CLA	CHC-C1C	2.62	1.41	1.35
31	g	613	CLA	CHC-C1C	2.62	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	608	CLA	CHC-C1C	2.62	1.41	1.35
31	b	603	CLA	CHC-C1C	2.62	1.41	1.35
31	b1	609	CLA	C3B-C2B	-2.61	1.36	1.40
31	s1	611	CLA	CHC-C1C	2.61	1.41	1.35
31	N	614	CLA	CHC-C1C	2.61	1.41	1.35
31	d1	402	CLA	CHC-C1C	2.61	1.41	1.35
31	B1	606	CLA	C3B-C2B	-2.61	1.36	1.40
31	B	616	CLA	CHC-C1C	2.61	1.41	1.35
31	R	612	CLA	CHC-C1C	2.61	1.41	1.35
31	d	402	CLA	C3B-C2B	-2.61	1.36	1.40
31	b	611	CLA	CHC-C1C	2.61	1.41	1.35
31	b	604	CLA	C3B-C2B	-2.61	1.36	1.40
31	N1	611	CLA	CHC-C1C	2.60	1.41	1.35
31	S1	602	CLA	CHC-C1C	2.60	1.41	1.35
31	C	505	CLA	CHC-C1C	2.60	1.41	1.35
31	S1	611	CLA	C3B-C2B	-2.60	1.36	1.40
31	Y	612	CLA	CHC-C1C	2.60	1.41	1.35
31	S	605	CLA	C3B-C2B	-2.60	1.36	1.40
31	b	602	CLA	CHC-C1C	2.60	1.41	1.35
31	n	610	CLA	CHC-C1C	2.60	1.41	1.35
31	G1	604	CLA	CHC-C1C	2.60	1.41	1.35
31	s1	617	CLA	CHC-C1C	2.60	1.41	1.35
35	J	101	LMG	C37-C36	-2.60	1.33	1.51
31	R1	603	CLA	CHC-C1C	2.60	1.41	1.35
31	y1	614	CLA	CHC-C1C	2.60	1.41	1.35
31	d	403	CLA	C3B-C2B	-2.60	1.36	1.40
31	C	511	CLA	CHC-C1C	2.60	1.41	1.35
31	G1	603	CLA	C3B-C2B	-2.60	1.36	1.40
31	s	611	CLA	CHC-C1C	2.60	1.41	1.35
31	R1	608	CLA	CHC-C1C	2.60	1.41	1.35
31	Y	611	CLA	CHC-C1C	2.60	1.41	1.35
31	n1	604	CLA	CHC-C1C	2.59	1.41	1.35
31	Y1	610	CLA	CHC-C1C	2.59	1.41	1.35
31	b1	616	CLA	CHC-C1C	2.59	1.41	1.35
31	R1	609	CLA	CHC-C1C	2.59	1.41	1.35
37	b1	620	C7Z	C21-C26	-2.59	1.50	1.53
31	C1	503	CLA	CHC-C1C	2.59	1.41	1.35
31	C	513	CLA	CHC-C1C	2.59	1.41	1.35
31	s	605	CLA	CHC-C1C	2.59	1.41	1.35
31	s	602	CLA	CHC-C1C	2.59	1.41	1.35
35	j	101	LMG	C37-C36	-2.59	1.33	1.51
31	N1	603	CLA	C3B-C2B	-2.59	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r1	625	LMT	O3'-C3'	-2.58	1.36	1.43
31	b	614	CLA	CHC-C1C	2.58	1.41	1.35
31	G1	614	CLA	CHC-C1C	2.58	1.41	1.35
31	R	608	CLA	CHC-C1C	2.58	1.41	1.35
31	Y1	611	CLA	CHC-C1C	2.58	1.41	1.35
31	r1	612	CLA	CHC-C1C	2.58	1.41	1.35
31	s1	603	CLA	CHC-C1C	2.58	1.41	1.35
31	B	602	CLA	CHC-C1C	2.58	1.41	1.35
31	Y	603	CLA	C3B-C2B	-2.58	1.36	1.40
31	b	610	CLA	CHC-C1C	2.58	1.41	1.35
31	c	503	CLA	CHC-C1C	2.58	1.41	1.35
31	C	502	CLA	C3B-C2B	-2.58	1.36	1.40
31	B1	603	CLA	CHC-C1C	2.58	1.41	1.35
31	B1	608	CLA	CHC-C1C	2.58	1.41	1.35
31	b1	614	CLA	CHC-C1C	2.58	1.41	1.35
32	A1	408	PHO	CAC-C3C	-2.58	1.47	1.52
31	G1	613	CLA	CHC-C1C	2.58	1.41	1.35
47	n1	606	CHL	C3B-C2B	-2.58	1.36	1.40
31	S	603	CLA	CHC-C1C	2.58	1.41	1.35
31	S1	605	CLA	CHC-C1C	2.58	1.41	1.35
31	Y	608	CLA	C3B-C2B	-2.57	1.36	1.40
31	r	608	CLA	C3B-C2B	-2.57	1.36	1.40
31	b1	607	CLA	CHC-C1C	2.57	1.41	1.35
31	N1	613	CLA	CHC-C1C	2.57	1.41	1.35
31	b	613	CLA	CHC-C1C	2.57	1.41	1.35
31	Y1	604	CLA	CHC-C1C	2.57	1.41	1.35
31	g1	612	CLA	CHC-C1C	2.57	1.41	1.35
31	D	403	CLA	C3B-C2B	-2.57	1.36	1.40
31	Y1	612	CLA	C3B-C2B	-2.57	1.36	1.40
31	C	501	CLA	CHC-C1C	2.57	1.41	1.35
31	a	407	CLA	CHC-C1C	2.57	1.41	1.35
31	c1	509	CLA	CHC-C1C	2.57	1.41	1.35
31	G	610	CLA	C3B-C2B	-2.57	1.36	1.40
31	s1	611	CLA	C3B-C2B	-2.57	1.36	1.40
31	N1	612	CLA	CHC-C1C	2.57	1.41	1.35
31	c	505	CLA	CHC-C1C	2.57	1.41	1.35
31	Y	610	CLA	C3B-C2B	-2.57	1.36	1.40
31	n	611	CLA	C3B-C2B	-2.57	1.36	1.40
31	Y1	608	CLA	CHC-C1C	2.57	1.41	1.35
31	Y	614	CLA	C3B-C2B	-2.57	1.36	1.40
35	D1	411	LMG	C37-C36	-2.57	1.33	1.51
47	N1	606	CHL	C3B-C2B	-2.56	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	512	CLA	CHC-C1C	2.56	1.41	1.35
31	S1	612	CLA	CHC-C1C	2.56	1.41	1.35
31	C	506	CLA	CHC-C1C	2.56	1.41	1.35
31	y	610	CLA	CHC-C1C	2.56	1.41	1.35
31	n1	603	CLA	CHC-C1C	2.56	1.41	1.35
31	r	603	CLA	CHC-C1C	2.56	1.41	1.35
31	N1	603	CLA	CHC-C1C	2.56	1.41	1.35
31	s1	609	CLA	CHC-C1C	2.56	1.41	1.35
31	S	613	CLA	CHC-C1C	2.56	1.41	1.35
31	c	512	CLA	CHC-C1C	2.56	1.41	1.35
31	B	614	CLA	CHC-C1C	2.56	1.41	1.35
31	G	612	CLA	C3B-C2B	-2.56	1.36	1.40
31	c1	506	CLA	CHC-C1C	2.56	1.41	1.35
31	g	603	CLA	C3B-C2B	-2.55	1.36	1.40
31	C1	506	CLA	CHC-C1C	2.55	1.41	1.35
31	R1	612	CLA	CHC-C1C	2.55	1.41	1.35
35	d	411	LMG	C37-C36	-2.55	1.33	1.51
31	s	604	CLA	CHC-C1C	2.55	1.41	1.35
31	c1	503	CLA	CHC-C1C	2.55	1.41	1.35
31	B	610	CLA	CHC-C1C	2.55	1.41	1.35
31	B1	602	CLA	CHC-C1C	2.55	1.41	1.35
31	G	602	CLA	CHC-C1C	2.55	1.41	1.35
31	N1	610	CLA	CHC-C1C	2.55	1.41	1.35
31	g1	603	CLA	CHC-C1C	2.55	1.41	1.35
31	y	613	CLA	CHC-C1C	2.55	1.41	1.35
31	y	612	CLA	C3B-C2B	-2.55	1.36	1.40
31	N	612	CLA	CHC-C1C	2.55	1.41	1.35
31	b1	615	CLA	C3B-C2B	-2.55	1.36	1.40
31	S	612	CLA	CHC-C1C	2.55	1.41	1.35
31	s1	605	CLA	CHC-C1C	2.55	1.41	1.35
31	S	605	CLA	CHC-C1C	2.55	1.41	1.35
31	r	608	CLA	CHC-C1C	2.55	1.41	1.35
31	c1	501	CLA	CHC-C1C	2.55	1.41	1.35
31	a1	406	CLA	CHC-C1C	2.54	1.41	1.35
31	C	504	CLA	CHC-C1C	2.54	1.41	1.35
31	B1	605	CLA	CHC-C1C	2.54	1.41	1.35
31	b1	611	CLA	CHC-C1C	2.54	1.41	1.35
31	S1	613	CLA	C3B-C2B	-2.54	1.36	1.40
31	c1	504	CLA	C3B-C2B	-2.54	1.36	1.40
52	i	101	3PH	O21-C2	-2.54	1.40	1.46
31	y	611	CLA	CHC-C1C	2.54	1.41	1.35
31	g1	603	CLA	C3B-C2B	-2.54	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B1	615	CLA	CHC-C1C	2.54	1.41	1.35
57	y1	627	PTY	O7-C6	-2.54	1.40	1.46
31	G	604	CLA	CHC-C1C	2.54	1.41	1.35
31	G	612	CLA	CHC-C1C	2.54	1.41	1.35
31	s1	613	CLA	C3B-C2B	-2.54	1.36	1.40
31	a1	405	CLA	CHC-C1C	2.54	1.41	1.35
31	R	611	CLA	C3B-C2B	-2.54	1.36	1.40
31	b	605	CLA	C3B-C2B	-2.54	1.36	1.40
31	Y	603	CLA	CHC-C1C	2.54	1.41	1.35
57	Y1	626	PTY	O7-C6	-2.54	1.40	1.46
35	d1	411	LMG	C37-C36	-2.54	1.33	1.51
31	B	607	CLA	CHC-C1C	2.54	1.41	1.35
31	C1	507	CLA	C3B-C2B	-2.54	1.36	1.40
56	R1	626	ERG	C14-C8	2.54	1.58	1.51
31	y	602	CLA	C1C-C2C	2.54	1.49	1.44
31	B	613	CLA	CHC-C1C	2.53	1.41	1.35
31	c	502	CLA	CHC-C1C	2.53	1.41	1.35
52	s	626	3PH	O21-C2	-2.53	1.40	1.46
31	B	615	CLA	CHC-C1C	2.53	1.41	1.35
31	Y1	612	CLA	CHC-C1C	2.53	1.41	1.35
31	s1	614	CLA	CHC-C1C	2.53	1.41	1.35
31	C1	505	CLA	CHC-C1C	2.53	1.41	1.35
31	Y	604	CLA	C3B-C2B	-2.53	1.36	1.40
35	D	411	LMG	C37-C36	-2.53	1.33	1.51
31	n1	602	CLA	CHC-C1C	2.53	1.41	1.35
31	s1	612	CLA	CHC-C1C	2.53	1.41	1.35
31	c	506	CLA	C3B-C2B	-2.53	1.36	1.40
31	b1	604	CLA	CHC-C1C	2.53	1.41	1.35
44	D	405	PL9	C53-C6	-2.53	1.45	1.50
31	Y1	603	CLA	C3B-C2B	-2.52	1.36	1.40
31	A	405	CLA	CHC-C1C	2.52	1.41	1.35
31	R1	604	CLA	CHC-C1C	2.52	1.41	1.35
32	A	408	PHO	CAC-C3C	-2.52	1.47	1.52
31	a	410	CLA	CHC-C1C	2.52	1.41	1.35
31	r1	604	CLA	CHC-C1C	2.52	1.41	1.35
31	B1	614	CLA	CHC-C1C	2.52	1.41	1.35
31	S1	617	CLA	CHC-C1C	2.52	1.41	1.35
49	r	622	XAT	O24-C25	-2.52	1.42	1.46
31	S1	603	CLA	C3B-C2B	-2.52	1.36	1.40
31	b1	603	CLA	CHC-C1C	2.52	1.41	1.35
31	b	604	CLA	CHC-C1C	2.52	1.41	1.35
31	y	608	CLA	C3B-C2B	-2.52	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	N	605	CHL	C3B-C2B	-2.52	1.36	1.40
31	s1	604	CLA	CHC-C1C	2.52	1.41	1.35
31	C1	501	CLA	CHC-C1C	2.52	1.41	1.35
31	r1	609	CLA	CHC-C1C	2.52	1.41	1.35
31	S	604	CLA	CHC-C1C	2.52	1.41	1.35
31	s1	610	CLA	CHC-C1C	2.52	1.41	1.35
47	s	601	CHL	C3B-C2B	-2.52	1.36	1.40
31	C1	511	CLA	CHC-C1C	2.52	1.41	1.35
31	S1	603	CLA	CHC-C1C	2.52	1.41	1.35
31	R1	612	CLA	C3B-C2B	-2.52	1.36	1.40
52	t1	101	3PH	O31-C31	2.51	1.40	1.33
31	y	614	CLA	C3B-C2B	-2.51	1.36	1.40
57	Y1	627	PTY	O7-C6	-2.51	1.40	1.46
31	y1	611	CLA	CHC-C1C	2.51	1.41	1.35
52	B1	624	3PH	O31-C31	2.51	1.40	1.33
31	B1	616	CLA	C3B-C2B	-2.51	1.36	1.40
31	A1	410	CLA	CHC-C1C	2.51	1.41	1.35
31	b1	612	CLA	CHC-C1C	2.51	1.41	1.35
31	C	503	CLA	C3B-C2B	-2.51	1.36	1.40
31	G1	611	CLA	CHC-C1C	2.51	1.41	1.35
31	c1	510	CLA	CHC-C1C	2.51	1.41	1.35
31	C1	501	CLA	C3B-C2B	-2.51	1.36	1.40
31	C	501	CLA	C3B-C2B	-2.51	1.36	1.40
31	C	510	CLA	C3B-C2B	-2.51	1.36	1.40
31	s1	603	CLA	C3B-C2B	-2.51	1.36	1.40
31	G	611	CLA	C3B-C2B	-2.51	1.36	1.40
52	S	626	3PH	O21-C2	-2.51	1.40	1.46
31	r1	603	CLA	CHC-C1C	2.50	1.41	1.35
31	S1	614	CLA	CHC-C1C	2.50	1.41	1.35
31	d	403	CLA	CHC-C1C	2.50	1.41	1.35
32	A1	409	PHO	CAC-C3C	-2.50	1.47	1.52
49	G	622	XAT	O24-C25	-2.50	1.42	1.46
31	y	612	CLA	CHC-C1C	2.50	1.41	1.35
31	G1	603	CLA	CHC-C1C	2.50	1.41	1.35
46	H1	101	RRX	C35-C13	2.50	1.56	1.50
31	C	510	CLA	CHC-C1C	2.50	1.41	1.35
31	y1	610	CLA	CHC-C1C	2.50	1.41	1.35
31	n	603	CLA	C3B-C2B	-2.50	1.36	1.40
37	b	620	C7Z	C18-C5	2.50	1.55	1.50
31	b1	609	CLA	CHC-C1C	2.50	1.41	1.35
31	s	614	CLA	CHC-C1C	2.50	1.41	1.35
52	s1	626	3PH	O21-C2	-2.50	1.40	1.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	604	CLA	C3B-C2B	-2.50	1.36	1.40
47	Y1	609	CHL	C3B-C2B	-2.50	1.36	1.40
31	y1	613	CLA	CHC-C1C	2.49	1.41	1.35
31	b1	602	CLA	C3B-C2B	-2.49	1.36	1.40
52	B1	624	3PH	O21-C2	-2.49	1.40	1.46
46	h1	101	RRX	C35-C13	2.49	1.56	1.50
31	C	502	CLA	CHC-C1C	2.49	1.41	1.35
31	a	407	CLA	C3B-C2B	-2.49	1.36	1.40
31	n1	611	CLA	C3B-C2B	-2.49	1.36	1.40
32	a1	409	PHO	CAC-C3C	-2.49	1.47	1.52
31	b1	610	CLA	CHC-C1C	2.49	1.41	1.35
31	y1	614	CLA	C3B-C2B	-2.49	1.36	1.40
31	n1	604	CLA	C3B-C2B	-2.49	1.36	1.40
31	a	405	CLA	CHC-C1C	2.48	1.41	1.35
31	A1	405	CLA	C1C-C2C	2.48	1.49	1.44
31	R	604	CLA	CHC-C1C	2.48	1.41	1.35
31	B	609	CLA	C3B-C2B	-2.48	1.36	1.40
31	B1	613	CLA	CHC-C1C	2.48	1.41	1.35
44	d1	405	PL9	C3-C4	-2.48	1.45	1.49
31	r1	603	CLA	C3B-C2B	-2.48	1.36	1.40
31	r	609	CLA	C3B-C2B	-2.48	1.36	1.40
37	B	620	C7Z	C21-C26	-2.48	1.50	1.53
31	Y	611	CLA	C3B-C2B	-2.48	1.36	1.40
31	A	410	CLA	CHC-C1C	2.47	1.41	1.35
31	B	617	CLA	CHC-C1C	2.47	1.41	1.35
31	B1	617	CLA	CHC-C1C	2.47	1.41	1.35
31	C	507	CLA	CHC-C1C	2.47	1.41	1.35
31	b	607	CLA	CHC-C1C	2.47	1.41	1.35
57	y1	626	PTY	O4-C30	2.47	1.40	1.33
31	g1	604	CLA	C3B-C2B	-2.47	1.36	1.40
31	g	603	CLA	CHC-C1C	2.47	1.41	1.35
37	B	620	C7Z	C18-C5	2.47	1.55	1.50
31	g1	612	CLA	C3B-C2B	-2.47	1.36	1.40
47	y	606	CHL	C3B-C2B	-2.47	1.36	1.40
52	S1	626	3PH	O21-C2	-2.47	1.40	1.46
31	s	613	CLA	CHC-C1C	2.47	1.41	1.35
31	r1	608	CLA	C3B-C2B	-2.47	1.36	1.40
31	y	614	CLA	CHC-C1C	2.46	1.41	1.35
31	s1	604	CLA	C3B-C2B	-2.46	1.36	1.40
31	y1	603	CLA	CHC-C1C	2.46	1.41	1.35
31	N	612	CLA	C3B-C2B	-2.46	1.36	1.40
31	r	613	CLA	CHC-C1C	2.46	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n1	603	CLA	C3B-C2B	-2.46	1.37	1.40
31	c	506	CLA	CHC-C1C	2.46	1.41	1.35
31	c1	504	CLA	CHC-C1C	2.46	1.41	1.35
31	D1	403	CLA	C3B-C2B	-2.46	1.37	1.40
49	G1	622	XAT	O24-C25	-2.46	1.42	1.46
31	D	402	CLA	C3B-C2B	-2.46	1.37	1.40
31	s	602	CLA	C3B-C2B	-2.46	1.37	1.40
31	b	617	CLA	CHC-C1C	2.46	1.41	1.35
31	B1	604	CLA	C3B-C2B	-2.46	1.37	1.40
31	S1	610	CLA	CHC-C1C	2.46	1.41	1.35
31	a1	407	CLA	CHC-C1C	2.46	1.41	1.35
31	r1	608	CLA	CHC-C1C	2.45	1.41	1.35
31	s	613	CLA	C3B-C2B	-2.45	1.37	1.40
52	b1	624	3PH	O31-C31	2.45	1.40	1.33
31	S	611	CLA	CHC-C1C	2.45	1.41	1.35
31	S	614	CLA	CHC-C1C	2.45	1.41	1.35
57	Y1	626	PTY	O4-C30	2.45	1.40	1.33
31	c1	502	CLA	CHC-C1C	2.45	1.41	1.35
31	N1	611	CLA	C3B-C2B	-2.45	1.37	1.40
31	c1	501	CLA	C3B-C2B	-2.45	1.37	1.40
31	N1	612	CLA	C3B-C2B	-2.45	1.37	1.40
31	A	407	CLA	CHC-C1C	2.45	1.41	1.35
31	B1	608	CLA	C3B-C2B	-2.45	1.37	1.40
52	t1	101	3PH	O21-C2	-2.44	1.40	1.46
31	S1	613	CLA	CHC-C1C	2.44	1.41	1.35
31	S1	609	CLA	C3B-C2B	-2.44	1.37	1.40
32	a	409	PHO	CAC-C3C	-2.44	1.48	1.52
31	C	506	CLA	C3B-C2B	-2.44	1.37	1.40
31	n	603	CLA	CHC-C1C	2.44	1.41	1.35
50	s	623	NEX	C1-C6	-2.44	1.50	1.54
31	c	507	CLA	C3B-C2B	-2.44	1.37	1.40
31	C	509	CLA	CHC-C1C	2.44	1.41	1.35
31	C	508	CLA	CHC-C1C	2.44	1.41	1.35
46	h	101	RRX	C35-C13	2.44	1.55	1.50
31	S	614	CLA	C3B-C2B	-2.44	1.37	1.40
31	y	611	CLA	C3B-C2B	-2.44	1.37	1.40
31	B1	609	CLA	CHC-C1C	2.44	1.41	1.35
31	A	410	CLA	C3B-C2B	-2.44	1.37	1.40
31	y	603	CLA	CHC-C1C	2.44	1.41	1.35
52	s1	626	3PH	O31-C31	2.43	1.40	1.33
55	R1	625	LMT	O2'-C2'	-2.43	1.37	1.43
49	g1	622	XAT	O24-C25	-2.43	1.42	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N1	614	CLA	C3B-C2B	-2.43	1.37	1.40
31	b1	615	CLA	CHC-C1C	2.43	1.41	1.35
31	s1	613	CLA	CHC-C1C	2.43	1.41	1.35
31	N	603	CLA	CHC-C1C	2.43	1.41	1.35
31	Y1	603	CLA	CHC-C1C	2.43	1.41	1.35
37	b	620	C7Z	C20-C13	2.43	1.55	1.50
31	B1	602	CLA	C3B-C2B	-2.43	1.37	1.40
31	c	508	CLA	CHC-C1C	2.43	1.41	1.35
52	s	626	3PH	O31-C31	2.42	1.40	1.33
31	B	604	CLA	C1C-C2C	2.42	1.49	1.44
31	S	612	CLA	C3B-C2B	-2.42	1.37	1.40
31	S1	604	CLA	CHC-C1C	2.42	1.41	1.35
31	b1	613	CLA	C1B-NB	2.42	1.37	1.35
31	c	504	CLA	CHC-C1C	2.42	1.41	1.35
57	y1	626	PTY	O7-C6	-2.42	1.40	1.46
31	Y	614	CLA	CHC-C1C	2.42	1.41	1.35
37	B1	620	C7Z	C20-C13	2.42	1.55	1.50
31	c	513	CLA	C3B-C2B	-2.42	1.37	1.40
31	B1	616	CLA	CHC-C1C	2.42	1.41	1.35
31	Y	612	CLA	C3B-C2B	-2.41	1.37	1.40
31	b1	604	CLA	C3B-C2B	-2.41	1.37	1.40
31	N1	604	CLA	CHC-C1C	2.41	1.41	1.35
37	b	620	C7Z	C21-C26	-2.41	1.50	1.53
31	y	602	CLA	C3B-C2B	-2.41	1.37	1.40
31	B	603	CLA	CHC-C1C	2.41	1.41	1.35
31	b1	613	CLA	CHC-C1C	2.41	1.41	1.35
31	B	611	CLA	C3B-C2B	-2.41	1.37	1.40
31	b	603	CLA	C3B-C2B	-2.41	1.37	1.40
31	b	611	CLA	C3B-C2B	-2.41	1.37	1.40
31	g1	614	CLA	C3B-C2B	-2.41	1.37	1.40
55	r1	625	LMT	O3B-C3B	-2.40	1.37	1.43
31	b1	602	CLA	CHC-C1C	2.40	1.41	1.35
52	S	626	3PH	O31-C31	2.40	1.40	1.33
31	a	406	CLA	CHC-C1C	2.40	1.41	1.35
31	b	616	CLA	CHC-C1C	2.40	1.41	1.35
31	B1	606	CLA	CHC-C1C	2.40	1.41	1.35
31	N	611	CLA	C3B-C2B	-2.40	1.37	1.40
31	s	609	CLA	C3B-C2B	-2.40	1.37	1.40
31	C1	507	CLA	CHC-C1C	2.40	1.41	1.35
31	b	611	CLA	C1C-C2C	2.40	1.49	1.44
47	N1	601	CHL	C3B-C2B	-2.40	1.37	1.40
47	S	601	CHL	C3B-C2B	-2.39	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S1	610	CLA	C3B-C2B	-2.39	1.37	1.40
31	S	613	CLA	C1A-CHA	2.39	1.53	1.43
31	Y1	614	CLA	C3B-C2B	-2.39	1.37	1.40
31	S	610	CLA	C1C-C2C	2.39	1.49	1.44
31	c	511	CLA	C3B-C2B	-2.39	1.37	1.40
31	R	612	CLA	C3B-C2B	-2.39	1.37	1.40
51	S1	625	LPX	P1-O2	2.38	1.68	1.59
46	H	101	RRX	C35-C13	2.38	1.55	1.50
50	n1	623	NEX	C17-C1	-2.38	1.49	1.53
49	R	621	XAT	O24-C25	-2.38	1.42	1.46
31	r	611	CLA	C3B-C2B	-2.38	1.37	1.40
31	g	613	CLA	C1C-C2C	2.38	1.49	1.44
31	C1	510	CLA	C3B-C2B	-2.38	1.37	1.40
31	b1	605	CLA	C1A-CHA	2.38	1.53	1.43
31	G1	602	CLA	C1C-C2C	2.38	1.49	1.44
31	S	604	CLA	C3B-C2B	-2.38	1.37	1.40
31	s1	603	CLA	C1A-CHA	2.38	1.53	1.43
31	y	604	CLA	CHC-C1C	2.37	1.41	1.35
47	G1	601	CHL	C3B-C2B	-2.37	1.37	1.40
31	A	406	CLA	CHC-C1C	2.37	1.41	1.35
31	C1	502	CLA	CHC-C1C	2.37	1.41	1.35
31	Y1	613	CLA	CHC-C1C	2.37	1.41	1.35
31	b	609	CLA	CHC-C1C	2.37	1.41	1.35
31	C1	510	CLA	CHC-C1C	2.37	1.41	1.35
31	B1	611	CLA	CHC-C1C	2.36	1.41	1.35
31	n1	613	CLA	C3B-C2B	-2.36	1.37	1.40
50	s	623	NEX	O4-C5	-2.36	1.39	1.43
47	g	601	CHL	C3B-C2B	-2.36	1.37	1.40
31	s	610	CLA	C1B-NB	2.36	1.37	1.35
31	C1	504	CLA	CHC-C1C	2.36	1.41	1.35
31	B1	617	CLA	C3B-C2B	-2.36	1.37	1.40
52	i	101	3PH	O31-C31	2.36	1.40	1.33
52	S1	626	3PH	O31-C31	2.36	1.40	1.33
37	b1	620	C7Z	C20-C13	2.36	1.55	1.50
52	b1	624	3PH	O21-C21	2.35	1.41	1.34
37	b1	620	C7Z	C18-C5	2.35	1.54	1.50
31	Y1	610	CLA	C3B-C2B	-2.35	1.37	1.40
31	b	608	CLA	C3B-C2B	-2.35	1.37	1.40
31	C1	512	CLA	C1C-C2C	2.35	1.49	1.44
31	n1	612	CLA	C1B-NB	2.35	1.37	1.35
52	T1	101	3PH	O21-C21	2.35	1.40	1.34
31	c	507	CLA	CHC-C1C	2.34	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	612	CLA	C3B-C2B	-2.34	1.37	1.40
31	C	504	CLA	C3B-C2B	-2.34	1.37	1.40
31	B1	603	CLA	C3B-C2B	-2.34	1.37	1.40
31	B1	609	CLA	C3B-C2B	-2.34	1.37	1.40
31	r1	602	CLA	C1C-C2C	2.34	1.49	1.44
31	s1	605	CLA	C3B-C2B	-2.34	1.37	1.40
31	y1	604	CLA	C3B-C2B	-2.34	1.37	1.40
52	T1	101	3PH	O31-C31	2.34	1.40	1.33
31	B	609	CLA	CHC-C1C	2.34	1.41	1.35
31	B1	605	CLA	C1A-CHA	2.34	1.52	1.43
31	n	613	CLA	C1B-NB	2.33	1.37	1.35
31	B	605	CLA	CHC-C1C	2.33	1.40	1.35
31	S1	617	CLA	C3B-C2B	-2.33	1.37	1.40
31	c1	506	CLA	C3B-C2B	-2.33	1.37	1.40
47	G1	608	CHL	C3B-C2B	-2.33	1.37	1.40
31	s1	602	CLA	C1C-C2C	2.33	1.49	1.44
47	G1	606	CHL	C3B-C2B	-2.33	1.37	1.40
31	S	603	CLA	C3B-C2B	-2.33	1.37	1.40
31	y1	611	CLA	C3B-C2B	-2.33	1.37	1.40
51	s1	625	LPX	P1-O2	2.33	1.68	1.59
31	b	610	CLA	C3B-C2B	-2.32	1.37	1.40
55	r1	625	LMT	O2B-C2B	-2.32	1.37	1.43
31	b	603	CLA	C1B-NB	2.32	1.37	1.35
52	b1	624	3PH	O21-C2	-2.32	1.40	1.46
49	g	622	XAT	O24-C25	-2.32	1.42	1.46
31	S1	605	CLA	C3B-C2B	-2.32	1.37	1.40
31	N	610	CLA	C3B-C2B	-2.32	1.37	1.40
31	n	611	CLA	C1B-NB	2.32	1.37	1.35
31	s1	605	CLA	C1A-CHA	2.32	1.52	1.43
31	B1	613	CLA	C3B-C2B	-2.32	1.37	1.40
31	B1	602	CLA	C1A-CHA	2.31	1.52	1.43
44	D1	405	PL9	C53-C6	-2.31	1.45	1.50
31	b	615	CLA	C1A-CHA	2.31	1.52	1.43
31	R1	608	CLA	C3B-C2B	-2.31	1.37	1.40
31	r1	610	CLA	C3B-C2B	-2.31	1.37	1.40
31	G	603	CLA	CHC-C1C	2.31	1.40	1.35
31	y	613	CLA	C3B-C2B	-2.31	1.37	1.40
31	B1	611	CLA	C3B-C2B	-2.31	1.37	1.40
31	G1	611	CLA	C3B-C2B	-2.31	1.37	1.40
47	R	606	CHL	C3B-C2B	-2.31	1.37	1.40
31	R	609	CLA	C1C-C2C	2.31	1.49	1.44
57	Y1	627	PTY	O7-C8	2.31	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R1	602	CLA	C1A-CHA	2.31	1.52	1.43
47	n	605	CHL	C3B-C2B	-2.31	1.37	1.40
31	B1	612	CLA	C1C-C2C	2.30	1.49	1.44
31	N	614	CLA	C3B-C2B	-2.30	1.37	1.40
31	b1	603	CLA	C3B-C2B	-2.30	1.37	1.40
31	c	513	CLA	C1C-C2C	2.30	1.49	1.44
31	C	507	CLA	C3B-C2B	-2.30	1.37	1.40
31	b	615	CLA	CHC-C1C	2.30	1.40	1.35
49	Y1	622	XAT	O24-C25	-2.30	1.42	1.46
31	n1	612	CLA	C3B-C2B	-2.30	1.37	1.40
31	G1	614	CLA	C3B-C2B	-2.30	1.37	1.40
47	s1	608	CHL	C3B-C2B	-2.30	1.37	1.40
31	s	609	CLA	C1C-C2C	2.30	1.49	1.44
44	d	405	PL9	C53-C6	-2.30	1.45	1.50
31	C	508	CLA	C3B-C2B	-2.30	1.37	1.40
31	s	605	CLA	C3B-C2B	-2.30	1.37	1.40
31	c1	502	CLA	C1A-CHA	2.29	1.52	1.43
51	s	625	LPX	P1-O2	2.29	1.68	1.59
55	r1	625	LMT	O4'-C4B	-2.29	1.37	1.43
31	a1	407	CLA	C1A-CHA	2.29	1.52	1.43
31	s	613	CLA	C1A-CHA	2.29	1.52	1.43
31	c1	508	CLA	C1C-C2C	2.29	1.49	1.44
31	b	617	CLA	C3B-C2B	-2.29	1.37	1.40
31	s1	609	CLA	C1A-CHA	2.29	1.52	1.43
31	G1	604	CLA	C3B-C2B	-2.29	1.37	1.40
31	C1	509	CLA	CHC-C1C	2.29	1.40	1.35
31	b1	610	CLA	C1A-CHA	2.29	1.52	1.43
49	r1	621	XAT	O24-C25	-2.29	1.42	1.46
55	R1	625	LMT	O2B-C2B	-2.29	1.37	1.43
31	r	603	CLA	C3B-C2B	-2.29	1.37	1.40
55	R1	625	LMT	O3B-C3B	-2.29	1.37	1.43
31	b	616	CLA	C3B-C2B	-2.28	1.37	1.40
31	s	604	CLA	C3B-C2B	-2.28	1.37	1.40
31	B	616	CLA	C1A-CHA	2.28	1.52	1.43
49	Y	622	XAT	O24-C25	-2.28	1.42	1.46
31	s	605	CLA	C1A-CHA	2.28	1.52	1.43
31	y1	613	CLA	C3B-C2B	-2.28	1.37	1.40
31	S1	614	CLA	C3B-C2B	-2.28	1.37	1.40
31	S1	603	CLA	C1A-CHA	2.28	1.52	1.43
31	C1	505	CLA	C3B-C2B	-2.28	1.37	1.40
31	r	610	CLA	C1C-C2C	2.28	1.49	1.44
31	r	610	CLA	C1A-CHA	2.28	1.52	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B1	620	C7Z	C18-C5	2.28	1.54	1.50
31	b1	614	CLA	C1C-C2C	2.28	1.49	1.44
31	b1	610	CLA	C3B-C2B	-2.28	1.37	1.40
31	S	609	CLA	C1C-C2C	2.28	1.49	1.44
31	B1	604	CLA	C1C-C2C	2.27	1.49	1.44
31	b1	611	CLA	C1C-C2C	2.27	1.49	1.44
31	B	610	CLA	C3B-C2B	-2.27	1.37	1.40
31	G1	613	CLA	C3B-C2B	-2.27	1.37	1.40
31	Y1	611	CLA	C3B-C2B	-2.27	1.37	1.40
31	g1	614	CLA	C1A-CHA	2.27	1.52	1.43
31	d	402	CLA	C1C-C2C	2.27	1.49	1.44
32	a1	409	PHO	CMD-C2D	-2.27	1.46	1.51
49	n	622	XAT	O24-C25	-2.27	1.43	1.46
31	N1	604	CLA	C3B-C2B	-2.27	1.37	1.40
31	s	610	CLA	C3B-C2B	-2.27	1.37	1.40
32	A	409	PHO	CMD-C2D	-2.27	1.46	1.51
31	b1	608	CLA	C1A-CHA	2.27	1.52	1.43
31	r	612	CLA	C1C-C2C	2.26	1.48	1.44
31	S1	605	CLA	C1A-CHA	2.26	1.52	1.43
31	b	605	CLA	C1A-CHA	2.26	1.52	1.43
47	G	609	CHL	C3A-C2A	-2.26	1.48	1.54
31	b1	602	CLA	C1A-CHA	2.26	1.52	1.43
37	B	620	C7Z	C20-C13	2.26	1.55	1.50
31	r	610	CLA	C3B-C2B	-2.26	1.37	1.40
31	b1	617	CLA	CHC-C1C	2.26	1.40	1.35
31	S1	602	CLA	C3B-C2B	-2.26	1.37	1.40
47	g1	608	CHL	C3B-C2B	-2.26	1.37	1.40
31	n1	613	CLA	C1A-CHA	2.26	1.52	1.43
31	c1	512	CLA	C1A-CHA	2.26	1.52	1.43
37	B	620	C7Z	C40-C33	2.26	1.55	1.50
31	n	611	CLA	C1C-C2C	2.26	1.48	1.44
31	b1	611	CLA	C3B-C2B	-2.26	1.37	1.40
31	y1	608	CLA	C3B-C2B	-2.26	1.37	1.40
31	R1	608	CLA	C1A-CHA	2.26	1.52	1.43
57	y1	626	PTY	O7-C8	2.26	1.40	1.34
31	G1	610	CLA	C1B-NB	2.26	1.37	1.35
49	N1	622	XAT	O24-C25	-2.26	1.43	1.46
31	y	608	CLA	C1C-C2C	2.26	1.48	1.44
31	a1	407	CLA	C3B-C2B	-2.26	1.37	1.40
31	B	607	CLA	C3B-C2B	-2.25	1.37	1.40
47	S1	601	CHL	C3B-C2B	-2.25	1.37	1.40
31	R	602	CLA	C1C-C2C	2.25	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	602	CLA	C1C-C2C	2.25	1.48	1.44
31	N1	614	CLA	C1C-C2C	2.25	1.48	1.44
31	b1	614	CLA	C1A-CHA	2.25	1.52	1.43
31	r	613	CLA	C1A-CHA	2.25	1.52	1.43
38	C1	524	DGA	OG2-CG2	-2.25	1.41	1.46
31	N	611	CLA	C1A-CHA	2.25	1.52	1.43
31	B	616	CLA	C3B-C2B	-2.25	1.37	1.40
51	S	625	LPX	P1-O2	2.25	1.68	1.59
49	y1	622	XAT	O24-C25	-2.25	1.43	1.46
31	g	611	CLA	C1A-CHA	2.25	1.52	1.43
55	r1	625	LMT	O2'-C2'	-2.25	1.37	1.43
31	R	603	CLA	C3B-C2B	-2.25	1.37	1.40
31	B	605	CLA	C1A-CHA	2.25	1.52	1.43
31	r1	612	CLA	C3B-C2B	-2.25	1.37	1.40
31	r1	608	CLA	C1A-CHA	2.25	1.52	1.43
31	b	605	CLA	CHC-C1C	2.25	1.40	1.35
31	s	612	CLA	C1C-C2C	2.24	1.48	1.44
31	n1	611	CLA	C1A-CHA	2.24	1.52	1.43
31	B1	610	CLA	C1C-C2C	2.24	1.48	1.44
31	n	613	CLA	C1C-C2C	2.24	1.48	1.44
31	R	611	CLA	C1C-C2C	2.24	1.48	1.44
31	n	612	CLA	C1C-C2C	2.24	1.48	1.44
31	g1	602	CLA	C1C-C2C	2.24	1.48	1.44
31	S1	611	CLA	CHC-C1C	2.24	1.40	1.35
31	n1	614	CLA	C1A-CHA	2.24	1.52	1.43
31	c1	507	CLA	C1C-C2C	2.24	1.48	1.44
31	s1	617	CLA	C1C-C2C	2.24	1.48	1.44
31	R	613	CLA	C3B-C2B	-2.24	1.37	1.40
31	S1	604	CLA	C3B-C2B	-2.24	1.37	1.40
31	b1	607	CLA	C3B-C2B	-2.24	1.37	1.40
31	n1	614	CLA	C1C-C2C	2.24	1.48	1.44
31	N	604	CLA	C1C-C2C	2.24	1.48	1.44
31	R1	612	CLA	C1A-CHA	2.24	1.52	1.43
32	a	409	PHO	CMC-C2C	-2.24	1.46	1.51
31	s	617	CLA	C1C-C2C	2.24	1.48	1.44
31	C1	506	CLA	C1A-CHA	2.24	1.52	1.43
31	R	613	CLA	C1C-C2C	2.24	1.48	1.44
31	d1	402	CLA	C1C-C2C	2.23	1.48	1.44
31	B	610	CLA	C1A-CHA	2.23	1.52	1.43
31	n	602	CLA	C1C-C2C	2.23	1.48	1.44
31	g1	610	CLA	C1C-C2C	2.23	1.48	1.44
49	N	622	XAT	O24-C25	-2.23	1.43	1.46

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	512	CLA	C1A-CHA	2.23	1.52	1.43
31	s1	610	CLA	C1A-CHA	2.23	1.52	1.43
31	g	602	CLA	C3B-C2B	-2.23	1.37	1.40
47	N1	608	CHL	C3A-C2A	-2.23	1.48	1.54
50	s1	623	NEX	C18-C5	2.23	1.56	1.52
31	g	613	CLA	C3B-C2B	-2.23	1.37	1.40
31	r	611	CLA	C1C-C2C	2.23	1.48	1.44
31	G1	614	CLA	C1A-CHA	2.23	1.52	1.43
31	r	611	CLA	C1A-CHA	2.23	1.52	1.43
31	Y1	608	CLA	C3B-C2B	-2.23	1.37	1.40
47	s	606	CHL	C3B-C2B	-2.23	1.37	1.40
31	S	611	CLA	C1A-CHA	2.23	1.52	1.43
31	s	605	CLA	C1C-C2C	2.23	1.48	1.44
31	b	615	CLA	CHD-C1D	2.23	1.42	1.38
31	n	614	CLA	C1C-C2C	2.23	1.48	1.44
31	R1	602	CLA	C3B-C2B	-2.23	1.37	1.40
31	R	603	CLA	C1A-CHA	2.23	1.52	1.43
31	R	608	CLA	C1A-CHA	2.23	1.52	1.43
57	y1	627	PTY	O7-C8	2.22	1.40	1.35
31	R	613	CLA	C1A-CHA	2.22	1.52	1.43
31	a	406	CLA	C1A-CHA	2.22	1.52	1.43
31	n	604	CLA	C1A-CHA	2.22	1.52	1.43
47	y1	606	CHL	C3B-C2B	-2.22	1.37	1.40
31	N1	602	CLA	C1C-C2C	2.22	1.48	1.44
31	n1	612	CLA	C1C-C2C	2.22	1.48	1.44
31	S1	611	CLA	C1A-CHA	2.22	1.52	1.43
31	b	608	CLA	C1A-CHA	2.22	1.52	1.43
31	n1	603	CLA	C1A-CHA	2.22	1.52	1.43
31	y1	610	CLA	C1A-CHA	2.22	1.52	1.43
31	y1	614	CLA	C1B-NB	2.22	1.37	1.35
31	c1	503	CLA	C1A-CHA	2.22	1.52	1.43
31	B	606	CLA	C3B-C2B	-2.22	1.37	1.40
31	c	511	CLA	C1C-C2C	2.22	1.48	1.44
31	r1	609	CLA	C3B-C2B	-2.22	1.37	1.40
31	c1	501	CLA	C1A-CHA	2.22	1.52	1.43
31	a1	406	CLA	C1A-CHA	2.22	1.52	1.43
47	n	606	CHL	CHC-C1C	2.22	1.40	1.35
31	y1	612	CLA	C3B-C2B	-2.21	1.37	1.40
31	c	509	CLA	CHC-C1C	2.21	1.40	1.35
31	b	602	CLA	C1A-CHA	2.21	1.52	1.43
31	s	603	CLA	C1A-CHA	2.21	1.52	1.43
31	c1	507	CLA	C3B-C2B	-2.21	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	613	CLA	C1A-CHA	2.21	1.52	1.43
31	g1	611	CLA	C3B-C2B	-2.21	1.37	1.40
31	G1	613	CLA	C1B-NB	2.21	1.37	1.35
31	b	616	CLA	C1A-CHA	2.21	1.52	1.43
31	r	602	CLA	C1A-CHA	2.21	1.52	1.43
31	B1	609	CLA	C1A-CHA	2.21	1.52	1.43
31	Y	613	CLA	C1C-C2C	2.21	1.48	1.44
31	B	609	CLA	C1A-CHA	2.21	1.52	1.43
31	b	607	CLA	C1A-CHA	2.21	1.52	1.43
31	a1	405	CLA	C1A-CHA	2.21	1.52	1.43
31	r1	612	CLA	C1A-CHA	2.21	1.52	1.43
31	Y1	602	CLA	C1C-C2C	2.21	1.48	1.44
49	n1	622	XAT	O24-C25	-2.21	1.43	1.46
31	A1	407	CLA	C1A-CHA	2.21	1.52	1.43
47	y1	609	CHL	C3B-C2B	-2.21	1.37	1.40
31	c1	511	CLA	C1C-C2C	2.21	1.48	1.44
52	t1	101	3PH	O21-C21	2.21	1.40	1.34
31	A	406	CLA	C1A-CHA	2.21	1.52	1.43
31	G	613	CLA	C1A-CHA	2.21	1.52	1.43
31	B	615	CLA	C1A-CHA	2.21	1.52	1.43
31	n1	614	CLA	C3B-C2B	-2.21	1.37	1.40
47	n1	601	CHL	C3B-C2B	-2.21	1.37	1.40
31	r1	612	CLA	MG-NC	2.21	2.11	2.06
31	S	605	CLA	C1A-CHA	2.21	1.52	1.43
31	c	513	CLA	C1B-NB	2.21	1.37	1.35
32	a	409	PHO	CMB-C2B	-2.21	1.46	1.51
31	n	611	CLA	C1A-CHA	2.21	1.52	1.43
31	g1	604	CLA	C1A-CHA	2.21	1.52	1.43
31	Y1	612	CLA	C1A-CHA	2.20	1.52	1.43
31	A1	410	CLA	C1A-CHA	2.20	1.52	1.43
31	S	609	CLA	C3B-C2B	-2.20	1.37	1.40
31	S	617	CLA	C1C-C2C	2.20	1.48	1.44
31	R1	610	CLA	C1C-C2C	2.20	1.48	1.44
31	N1	604	CLA	C3D-C4D	-2.20	1.39	1.44
31	G1	612	CLA	C1A-CHA	2.20	1.52	1.43
31	S1	610	CLA	C1A-CHA	2.20	1.52	1.43
31	g	613	CLA	C1A-CHA	2.20	1.52	1.43
47	Y	609	CHL	C3B-C2B	-2.20	1.37	1.40
31	G1	604	CLA	C1C-C2C	2.20	1.48	1.44
31	N1	603	CLA	C1A-CHA	2.20	1.52	1.43
31	s	612	CLA	C1B-NB	2.20	1.37	1.35
31	n	610	CLA	C3B-C2B	-2.20	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	611	CLA	C1C-C2C	2.20	1.48	1.44
31	c	505	CLA	C1A-CHA	2.20	1.52	1.43
47	N	601	CHL	C3B-C2B	-2.20	1.37	1.40
47	S1	608	CHL	C3B-C2B	-2.20	1.37	1.40
31	r	602	CLA	C1C-C2C	2.20	1.48	1.44
31	S	602	CLA	C3B-C2B	-2.20	1.37	1.40
31	d1	403	CLA	C1A-CHA	2.20	1.52	1.43
31	g1	611	CLA	C1A-CHA	2.20	1.52	1.43
31	r1	602	CLA	C1A-CHA	2.20	1.52	1.43
31	A1	407	CLA	C3B-C2B	-2.20	1.37	1.40
31	S	603	CLA	C1A-CHA	2.20	1.52	1.43
31	r	608	CLA	C1A-CHA	2.20	1.52	1.43
31	B1	607	CLA	C1A-CHA	2.19	1.52	1.43
31	Y1	602	CLA	C3B-C2B	-2.19	1.37	1.40
32	a	408	PHO	CMC-C2C	-2.19	1.46	1.51
31	c1	513	CLA	C1A-CHA	2.19	1.52	1.43
31	r1	612	CLA	C1B-NB	2.19	1.37	1.35
38	J1	101	DGA	OG2-CG2	-2.19	1.41	1.46
31	B	612	CLA	C1A-CHA	2.19	1.52	1.43
31	y1	608	CLA	C1A-CHA	2.19	1.52	1.43
31	c	510	CLA	C3B-C2B	-2.19	1.37	1.40
31	g1	602	CLA	C3B-C2B	-2.19	1.37	1.40
31	C	501	CLA	C3D-C4D	-2.19	1.39	1.44
31	N	602	CLA	C1C-C2C	2.19	1.48	1.44
31	R1	609	CLA	C1A-CHA	2.19	1.52	1.43
31	b	603	CLA	C1C-C2C	2.19	1.48	1.44
31	S1	604	CLA	C1A-CHA	2.19	1.52	1.43
31	b	613	CLA	C3D-C4D	-2.19	1.39	1.44
31	c1	505	CLA	C1C-C2C	2.19	1.48	1.44
31	g	612	CLA	C1C-C2C	2.19	1.48	1.44
31	C1	505	CLA	C1A-CHA	2.19	1.52	1.43
31	R	611	CLA	C1B-NB	2.19	1.37	1.35
37	b	620	C7Z	C40-C33	2.19	1.55	1.50
31	s	611	CLA	C1A-CHA	2.19	1.52	1.43
31	y	610	CLA	C1A-CHA	2.19	1.52	1.43
31	B1	614	CLA	C1A-CHA	2.19	1.52	1.43
31	c	509	CLA	C1A-CHA	2.19	1.52	1.43
31	y	612	CLA	C1A-CHA	2.19	1.52	1.43
31	G1	612	CLA	C1C-C2C	2.19	1.48	1.44
52	S	626	3PH	O21-C21	2.19	1.40	1.34
31	N	613	CLA	C1A-CHA	2.18	1.52	1.43
31	c1	509	CLA	C1A-CHA	2.18	1.52	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g1	613	CLA	C1A-CHA	2.18	1.52	1.43
31	G1	614	CLA	C1C-C2C	2.18	1.48	1.44
31	B1	615	CLA	C1A-CHA	2.18	1.52	1.43
31	y1	613	CLA	C1A-CHA	2.18	1.52	1.43
31	s1	613	CLA	C1A-CHA	2.18	1.52	1.43
49	y	622	XAT	O24-C25	-2.18	1.43	1.46
31	b	607	CLA	C3D-C4D	-2.18	1.39	1.44
47	r	606	CHL	C3B-C2B	-2.18	1.37	1.40
37	b1	620	C7Z	C40-C33	2.18	1.55	1.50
31	b	604	CLA	C1A-CHA	2.18	1.52	1.43
31	S	604	CLA	C1A-CHA	2.18	1.52	1.43
31	R	608	CLA	C1B-NB	2.18	1.37	1.35
31	r1	610	CLA	C1C-C2C	2.18	1.48	1.44
31	n1	614	CLA	C1B-NB	2.18	1.37	1.35
31	Y	610	CLA	C1A-CHA	2.18	1.52	1.43
31	g1	612	CLA	C1A-CHA	2.18	1.52	1.43
52	S1	626	3PH	O31-C3	-2.18	1.40	1.45
47	r	607	CHL	C3B-C2B	-2.18	1.37	1.40
31	s	602	CLA	C1A-CHA	2.18	1.52	1.43
31	r1	604	CLA	C1A-CHA	2.18	1.52	1.43
31	c1	513	CLA	C1C-C2C	2.18	1.48	1.44
31	S1	617	CLA	C1C-C2C	2.18	1.48	1.44
31	N	613	CLA	C1C-C2C	2.18	1.48	1.44
31	s1	614	CLA	C1A-CHA	2.18	1.52	1.43
31	N1	614	CLA	C1A-CHA	2.18	1.52	1.43
31	b1	616	CLA	C1C-C2C	2.18	1.48	1.44
31	c	501	CLA	C3D-C4D	-2.17	1.39	1.44
31	s1	617	CLA	C1A-CHA	2.17	1.52	1.43
31	g1	614	CLA	C1C-C2C	2.17	1.48	1.44
31	R	603	CLA	C1C-C2C	2.17	1.48	1.44
31	b1	615	CLA	C1A-CHA	2.17	1.52	1.43
31	y1	612	CLA	C1C-C2C	2.17	1.48	1.44
32	A	409	PHO	CMC-C2C	-2.17	1.46	1.51
31	N	610	CLA	C1C-C2C	2.17	1.48	1.44
52	B1	624	3PH	O21-C21	2.17	1.40	1.34
31	n	610	CLA	C1A-CHA	2.17	1.52	1.43
31	S1	617	CLA	C1A-CHA	2.17	1.52	1.43
38	c1	524	DGA	OG2-CG2	-2.17	1.41	1.46
31	y1	612	CLA	C1A-CHA	2.17	1.52	1.43
31	g	604	CLA	C1C-C2C	2.17	1.48	1.44
31	c	508	CLA	C1A-CHA	2.17	1.52	1.43
31	b	606	CLA	CHC-C1C	2.17	1.40	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y1	604	CLA	C1A-CHA	2.17	1.52	1.43
31	s1	614	CLA	C3B-C2B	-2.17	1.37	1.40
31	g1	613	CLA	C1C-C2C	2.17	1.48	1.44
31	C	511	CLA	C1A-CHA	2.17	1.52	1.43
31	S1	609	CLA	C1A-CHA	2.17	1.52	1.43
31	A1	406	CLA	C1C-C2C	2.17	1.48	1.44
31	B	613	CLA	C3D-C4D	-2.17	1.39	1.44
31	r1	603	CLA	C1A-CHA	2.17	1.52	1.43
31	s1	604	CLA	C1A-CHA	2.17	1.52	1.43
31	G	611	CLA	C1A-CHA	2.17	1.52	1.43
31	s	614	CLA	C1A-CHA	2.17	1.52	1.43
31	G	612	CLA	C1A-CHA	2.16	1.52	1.43
31	b1	613	CLA	C1A-CHA	2.16	1.52	1.43
31	y	603	CLA	C1A-CHA	2.16	1.52	1.43
31	N1	611	CLA	C1A-CHA	2.16	1.52	1.43
31	S	603	CLA	C1C-C2C	2.16	1.48	1.44
32	a1	408	PHO	CMC-C2C	-2.16	1.46	1.51
47	Y	606	CHL	C3B-C2B	-2.16	1.37	1.40
52	T1	101	3PH	O31-C3	-2.16	1.40	1.45
31	n1	610	CLA	C1A-CHA	2.16	1.52	1.43
31	R1	608	CLA	C1C-C2C	2.16	1.48	1.44
52	S	626	3PH	O31-C3	-2.16	1.40	1.45
31	c	509	CLA	C3B-C2B	-2.16	1.37	1.40
31	r	603	CLA	C1A-CHA	2.16	1.52	1.43
31	n	614	CLA	C1A-CHA	2.16	1.52	1.43
31	Y	611	CLA	C1A-CHA	2.16	1.52	1.43
31	b1	617	CLA	C1A-CHA	2.16	1.52	1.43
37	B1	620	C7Z	C40-C33	2.16	1.55	1.50
31	S	612	CLA	C1A-CHA	2.16	1.52	1.43
52	i	101	3PH	O21-C21	2.16	1.40	1.34
31	n1	612	CLA	C1A-CHA	2.16	1.52	1.43
31	y	611	CLA	C1A-CHA	2.16	1.52	1.43
31	N1	613	CLA	C1A-CHA	2.16	1.52	1.43
31	a	410	CLA	C1A-CHA	2.16	1.52	1.43
31	C1	511	CLA	C1A-CHA	2.16	1.52	1.43
31	B	606	CLA	C1C-C2C	2.16	1.48	1.44
56	r1	626	ERG	C14-C8	2.16	1.57	1.51
31	g	612	CLA	C1A-CHA	2.16	1.52	1.43
31	s1	612	CLA	C1A-CHA	2.16	1.52	1.43
31	r1	609	CLA	C1B-NB	2.16	1.37	1.35
32	a1	409	PHO	CMC-C2C	-2.16	1.46	1.51
31	B	602	CLA	C1A-CHA	2.16	1.52	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y1	611	CLA	C1A-CHA	2.16	1.52	1.43
31	S	609	CLA	C1A-CHA	2.15	1.52	1.43
31	B1	611	CLA	C1A-CHA	2.15	1.52	1.43
31	c1	505	CLA	C1A-CHA	2.15	1.52	1.43
31	S	602	CLA	C1A-CHA	2.15	1.52	1.43
31	B1	608	CLA	C1A-CHA	2.15	1.52	1.43
31	R1	604	CLA	C1A-CHA	2.15	1.52	1.43
31	y1	602	CLA	C1A-CHA	2.15	1.52	1.43
31	c1	504	CLA	C1A-CHA	2.15	1.52	1.43
31	s	603	CLA	C3B-C2B	-2.15	1.37	1.40
31	g	602	CLA	C1C-C2C	2.15	1.48	1.44
31	R1	603	CLA	C1C-C2C	2.15	1.48	1.44
31	n1	613	CLA	C1C-C2C	2.15	1.48	1.44
32	A1	409	PHO	CMB-C2B	-2.15	1.46	1.51
31	b	609	CLA	C3D-C4D	-2.15	1.39	1.44
31	R	613	CLA	C1B-NB	2.15	1.37	1.35
31	s	609	CLA	C1B-NB	2.15	1.37	1.35
31	g1	603	CLA	C1C-C2C	2.15	1.48	1.44
31	r	612	CLA	C1A-CHA	2.15	1.52	1.43
31	d1	403	CLA	C1C-C2C	2.15	1.48	1.44
50	S1	623	NEX	O4-C5	2.15	1.47	1.43
31	b1	616	CLA	C1A-CHA	2.15	1.52	1.43
31	B	614	CLA	C1A-CHA	2.15	1.52	1.43
31	c	507	CLA	C1A-CHA	2.15	1.52	1.43
31	A	405	CLA	C3D-C4D	-2.15	1.39	1.44
31	C1	509	CLA	C1A-CHA	2.15	1.52	1.43
31	r1	604	CLA	C3B-C2B	-2.15	1.37	1.40
31	B	603	CLA	C1A-CHA	2.15	1.52	1.43
31	B1	605	CLA	C3B-C2B	-2.15	1.37	1.40
31	N1	613	CLA	C1C-C2C	2.15	1.48	1.44
31	Y1	608	CLA	C1C-C2C	2.15	1.48	1.44
31	a	407	CLA	C1A-CHA	2.15	1.52	1.43
31	g1	610	CLA	C1A-CHA	2.15	1.52	1.43
31	A	407	CLA	C1A-CHA	2.15	1.52	1.43
31	B	607	CLA	C1A-CHA	2.15	1.52	1.43
31	n	614	CLA	C3B-C2B	-2.15	1.37	1.40
31	c1	513	CLA	C3B-C2B	-2.15	1.37	1.40
31	g	614	CLA	C1A-CHA	2.15	1.52	1.43
31	C	503	CLA	C1A-CHA	2.15	1.52	1.43
31	R1	610	CLA	C1A-CHA	2.15	1.52	1.43
31	Y1	610	CLA	C1A-CHA	2.15	1.52	1.43
31	c1	506	CLA	C1A-CHA	2.15	1.52	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	602	CLA	C1A-CHA	2.15	1.52	1.43
31	n	603	CLA	C1A-CHA	2.15	1.52	1.43
31	n	614	CLA	C1B-NB	2.15	1.37	1.35
31	N	612	CLA	C1C-C2C	2.15	1.48	1.44
31	N	612	CLA	C1A-CHA	2.15	1.52	1.43
31	c1	502	CLA	C3B-C2B	-2.14	1.37	1.40
31	s1	603	CLA	C1C-C2C	2.14	1.48	1.44
31	g	614	CLA	C1C-C2C	2.14	1.48	1.44
31	C	503	CLA	C1C-C2C	2.14	1.48	1.44
31	B1	615	CLA	C3B-C2B	-2.14	1.37	1.40
31	C	512	CLA	C1A-CHA	2.14	1.52	1.43
31	b1	604	CLA	C1A-CHA	2.14	1.52	1.43
31	b1	609	CLA	C1A-CHA	2.14	1.52	1.43
31	N	614	CLA	C1B-NB	2.14	1.37	1.35
32	a	408	PHO	CMD-C2D	-2.14	1.46	1.51
31	b	606	CLA	C1A-CHA	2.14	1.52	1.43
31	A1	406	CLA	C1A-CHA	2.14	1.52	1.43
52	s1	626	3PH	O21-C21	2.14	1.40	1.34
31	C	502	CLA	C1A-CHA	2.14	1.52	1.43
52	S1	626	3PH	O21-C21	2.14	1.40	1.34
31	D1	403	CLA	C1C-C2C	2.14	1.48	1.44
31	Y1	614	CLA	C1C-C2C	2.14	1.48	1.44
52	s	626	3PH	O21-C21	2.14	1.40	1.34
47	y1	605	CHL	C3B-C2B	-2.14	1.37	1.40
31	r1	609	CLA	C1A-CHA	2.14	1.52	1.43
31	c1	501	CLA	C1C-C2C	2.14	1.48	1.44
31	B1	606	CLA	C1A-CHA	2.14	1.52	1.43
31	b1	603	CLA	C1A-CHA	2.14	1.52	1.43
31	N1	613	CLA	C3B-C2B	-2.14	1.37	1.40
31	n1	604	CLA	C1A-CHA	2.14	1.52	1.43
31	g	612	CLA	C1B-NB	2.14	1.37	1.35
31	s	603	CLA	C1C-C2C	2.14	1.48	1.44
31	Y1	608	CLA	C3D-C4D	-2.14	1.39	1.44
31	B1	615	CLA	C1C-C2C	2.14	1.48	1.44
31	R1	612	CLA	C1C-C2C	2.14	1.48	1.44
31	A	410	CLA	C1A-CHA	2.14	1.52	1.43
31	C1	502	CLA	C1A-CHA	2.14	1.52	1.43
31	C1	512	CLA	C1A-CHA	2.14	1.52	1.43
31	G1	611	CLA	C1A-CHA	2.14	1.52	1.43
31	a1	410	CLA	C1A-CHA	2.14	1.52	1.43
31	c1	510	CLA	C1A-CHA	2.14	1.52	1.43
31	y	608	CLA	C1A-CHA	2.14	1.52	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b1	612	CLA	C1A-CHA	2.14	1.52	1.43
31	s1	605	CLA	MG-NC	2.14	2.11	2.06
31	c	503	CLA	C1A-CHA	2.14	1.52	1.43
31	C	511	CLA	C1C-C2C	2.14	1.48	1.44
31	B	609	CLA	C3D-C4D	-2.13	1.39	1.44
31	C	505	CLA	C1A-CHA	2.13	1.52	1.43
31	S1	602	CLA	C1A-CHA	2.13	1.52	1.43
56	R1	626	ERG	C11-C9	2.13	1.57	1.53
31	G	603	CLA	C1A-CHA	2.13	1.52	1.43
31	R	610	CLA	C1A-CHA	2.13	1.52	1.43
31	b	614	CLA	C1A-CHA	2.13	1.52	1.43
31	r	604	CLA	C3B-C2B	-2.13	1.37	1.40
31	n1	602	CLA	C3B-C2B	-2.13	1.37	1.40
31	A1	407	CLA	C1C-C2C	2.13	1.48	1.44
31	g1	602	CLA	C1A-CHA	2.13	1.51	1.43
31	y1	604	CLA	C1C-C2C	2.13	1.48	1.44
31	D	403	CLA	C1B-NB	2.13	1.37	1.35
31	g	614	CLA	C3B-C2B	-2.13	1.37	1.40
47	S	607	CHL	C3B-C2B	-2.13	1.37	1.40
31	B	608	CLA	C1A-CHA	2.13	1.51	1.43
31	G	610	CLA	C1A-CHA	2.13	1.51	1.43
31	s1	611	CLA	C1C-C2C	2.13	1.48	1.44
31	B1	603	CLA	C1A-CHA	2.13	1.51	1.43
31	R	612	CLA	C1A-CHA	2.13	1.51	1.43
31	B	611	CLA	C1C-C2C	2.13	1.48	1.44
31	n	602	CLA	C1A-CHA	2.13	1.51	1.43
31	r	609	CLA	C1A-CHA	2.13	1.51	1.43
31	A1	405	CLA	C1A-CHA	2.13	1.51	1.43
31	y1	611	CLA	C3D-C4D	-2.13	1.39	1.44
31	g1	603	CLA	C1A-CHA	2.13	1.51	1.43
31	B1	616	CLA	C1A-CHA	2.13	1.51	1.43
31	c	513	CLA	C1A-CHA	2.13	1.51	1.43
31	n1	611	CLA	C1C-C2C	2.13	1.48	1.44
31	s	617	CLA	C1A-CHA	2.13	1.51	1.43
31	B	610	CLA	C1C-C2C	2.13	1.48	1.44
31	R	611	CLA	C1A-CHA	2.13	1.51	1.43
49	R1	621	XAT	O24-C25	-2.12	1.43	1.46
31	C1	510	CLA	C3D-C4D	-2.12	1.39	1.44
31	R1	603	CLA	C1A-CHA	2.12	1.51	1.43
31	s1	602	CLA	C3B-C2B	-2.12	1.37	1.40
31	g	604	CLA	C1A-CHA	2.12	1.51	1.43
31	c	510	CLA	C3D-C4D	-2.12	1.39	1.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C1	504	CLA	C1A-CHA	2.12	1.51	1.43
32	A1	409	PHO	CMC-C2C	-2.12	1.46	1.51
31	G	602	CLA	C1A-CHA	2.12	1.51	1.43
31	b1	611	CLA	C1A-CHA	2.12	1.51	1.43
31	S1	602	CLA	C1C-C2C	2.12	1.48	1.44
31	y1	608	CLA	C1C-C2C	2.12	1.48	1.44
31	S	602	CLA	C1B-NB	2.12	1.37	1.35
31	Y1	611	CLA	C1A-CHA	2.12	1.51	1.43
31	D	403	CLA	C1C-C2C	2.12	1.48	1.44
47	s	608	CHL	C3B-C2B	-2.12	1.37	1.40
31	b1	607	CLA	C1A-CHA	2.12	1.51	1.43
31	G	614	CLA	C1C-C2C	2.12	1.48	1.44
31	G	614	CLA	C1A-CHA	2.12	1.51	1.43
31	y	613	CLA	C1A-CHA	2.12	1.51	1.43
31	g	611	CLA	C3B-C2B	-2.12	1.37	1.40
31	C	513	CLA	C1A-CHA	2.12	1.51	1.43
31	C1	513	CLA	C1A-CHA	2.12	1.51	1.43
31	s1	611	CLA	C1A-CHA	2.12	1.51	1.43
31	N	603	CLA	C1A-CHA	2.12	1.51	1.43
31	N	604	CLA	C1A-CHA	2.12	1.51	1.43
31	R	610	CLA	C1C-C2C	2.12	1.48	1.44
31	G1	604	CLA	C1A-CHA	2.12	1.51	1.43
31	s	617	CLA	C1B-NB	2.12	1.37	1.35
31	Y1	613	CLA	C1A-CHA	2.12	1.51	1.43
31	S	617	CLA	C1A-CHA	2.12	1.51	1.43
31	r1	603	CLA	C1C-C2C	2.12	1.48	1.44
31	y	604	CLA	C1A-CHA	2.12	1.51	1.43
31	N1	612	CLA	C1A-CHA	2.12	1.51	1.43
31	S1	614	CLA	C1A-CHA	2.12	1.51	1.43
31	b	609	CLA	C1A-CHA	2.12	1.51	1.43
31	c	504	CLA	C1A-CHA	2.11	1.51	1.43
31	B	617	CLA	C3D-C4D	-2.11	1.39	1.44
31	Y	608	CLA	C1A-CHA	2.11	1.51	1.43
31	r1	610	CLA	C1A-CHA	2.11	1.51	1.43
33	c1	515	BCR	C12-C13	-2.11	1.41	1.45
31	y1	602	CLA	C1C-C2C	2.11	1.48	1.44
31	c1	511	CLA	C1A-CHA	2.11	1.51	1.43
47	G	609	CHL	C3B-C2B	-2.11	1.37	1.40
52	i	101	3PH	O31-C3	-2.11	1.40	1.45
50	s1	623	NEX	C17-C1	-2.11	1.49	1.53
31	G	604	CLA	C1C-C2C	2.11	1.48	1.44
31	Y	612	CLA	C1C-C2C	2.11	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C1	501	CLA	C1A-CHA	2.11	1.51	1.43
31	a	407	CLA	C3D-C4D	-2.11	1.39	1.44
31	G1	613	CLA	C1A-CHA	2.11	1.51	1.43
31	N	614	CLA	C1C-C2C	2.11	1.48	1.44
31	g	603	CLA	C1C-C2C	2.11	1.48	1.44
31	a	410	CLA	C3B-C2B	-2.11	1.37	1.40
31	G1	610	CLA	C3B-C2B	-2.11	1.37	1.40
31	y1	610	CLA	C3B-C2B	-2.11	1.37	1.40
31	b1	603	CLA	C1C-C2C	2.11	1.48	1.44
31	s	610	CLA	C1A-CHA	2.11	1.51	1.43
31	y	614	CLA	C1A-CHA	2.11	1.51	1.43
31	N	604	CLA	C3B-C2B	-2.11	1.37	1.40
31	N	614	CLA	C1A-CHA	2.11	1.51	1.43
31	S	610	CLA	C1A-CHA	2.11	1.51	1.43
31	B1	610	CLA	C1A-CHA	2.11	1.51	1.43
31	g	611	CLA	C1C-C2C	2.11	1.48	1.44
31	C1	513	CLA	C1C-C2C	2.11	1.48	1.44
31	G	611	CLA	C1B-NB	2.11	1.37	1.35
31	B1	603	CLA	C1B-NB	2.11	1.37	1.35
31	D	403	CLA	C1A-CHA	2.10	1.51	1.43
31	g	603	CLA	C1A-CHA	2.10	1.51	1.43
31	N	610	CLA	C1B-NB	2.10	1.37	1.35
31	A	410	CLA	C1B-NB	2.10	1.37	1.35
31	D1	403	CLA	C1A-CHA	2.10	1.51	1.43
38	j1	101	DGA	OG2-CG2	-2.10	1.41	1.46
31	s	605	CLA	MG-NC	2.10	2.11	2.06
31	Y1	614	CLA	C3D-C4D	-2.10	1.39	1.44
31	d	403	CLA	C1A-CHA	2.10	1.51	1.43
31	c	506	CLA	C1A-CHA	2.10	1.51	1.43
31	G	613	CLA	C3B-C2B	-2.10	1.37	1.40
45	F1	101	HEM	CMB-C2B	2.10	1.55	1.50
31	N1	612	CLA	C1C-C2C	2.10	1.48	1.44
45	f1	101	HEM	CMB-C2B	2.10	1.55	1.50
31	G	612	CLA	C1C-C2C	2.10	1.48	1.44
31	Y	604	CLA	C1C-C2C	2.10	1.48	1.44
31	c	512	CLA	C1C-C2C	2.10	1.48	1.44
38	c	524	DGA	OG2-CG2	-2.10	1.41	1.46
31	R	603	CLA	MG-NC	2.10	2.11	2.06
31	A1	410	CLA	C1C-C2C	2.10	1.48	1.44
31	s	604	CLA	C1A-CHA	2.10	1.51	1.43
31	S	614	CLA	C1A-CHA	2.10	1.51	1.43
31	n	613	CLA	C1A-CHA	2.10	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	613	CLA	C1C-C2C	2.10	1.48	1.44
31	b	603	CLA	C1A-CHA	2.10	1.51	1.43
31	r	611	CLA	C1B-NB	2.10	1.37	1.35
52	s1	626	3PH	O31-C3	-2.10	1.40	1.45
31	Y1	604	CLA	C1A-CHA	2.10	1.51	1.43
31	c	501	CLA	C1C-C2C	2.09	1.48	1.44
47	g1	601	CHL	C3B-C2B	-2.09	1.37	1.40
47	Y1	606	CHL	C3A-C2A	-2.09	1.48	1.54
31	b	611	CLA	C1A-CHA	2.09	1.51	1.43
31	R	609	CLA	C1A-CHA	2.09	1.51	1.43
31	C1	508	CLA	C1A-CHA	2.09	1.51	1.43
38	C	524	DGA	OG2-CG2	-2.09	1.41	1.46
32	a1	409	PHO	CMB-C2B	-2.09	1.46	1.51
31	S1	609	CLA	C1B-NB	2.09	1.37	1.35
55	R1	625	LMT	O4'-C4B	-2.09	1.38	1.43
31	Y	608	CLA	C1C-C2C	2.09	1.48	1.44
31	s1	604	CLA	C1C-C2C	2.09	1.48	1.44
31	Y1	608	CLA	C1A-CHA	2.09	1.51	1.43
31	c	510	CLA	C1C-C2C	2.09	1.48	1.44
31	S1	609	CLA	C3D-C4D	-2.09	1.39	1.44
31	G	604	CLA	C1A-CHA	2.09	1.51	1.43
31	c1	507	CLA	C1A-CHA	2.09	1.51	1.43
52	s	626	3PH	O31-C3	-2.09	1.40	1.45
31	r	603	CLA	C1C-C2C	2.09	1.48	1.44
31	C1	501	CLA	C1C-C2C	2.09	1.48	1.44
31	B	604	CLA	C3D-C4D	-2.09	1.39	1.44
31	c	512	CLA	C3B-C2B	-2.09	1.37	1.40
31	B1	617	CLA	C1A-CHA	2.09	1.51	1.43
31	C1	503	CLA	C1A-CHA	2.09	1.51	1.43
31	c	502	CLA	C1A-CHA	2.09	1.51	1.43
31	S1	613	CLA	C1A-CHA	2.09	1.51	1.43
31	C	513	CLA	C1C-C2C	2.09	1.48	1.44
31	B1	602	CLA	C1C-C2C	2.09	1.48	1.44
31	r1	604	CLA	C1B-NB	2.09	1.37	1.35
31	r	604	CLA	C1A-CHA	2.09	1.51	1.43
32	a	408	PHO	CMB-C2B	-2.09	1.46	1.51
31	C	505	CLA	C1C-C2C	2.09	1.48	1.44
31	R	612	CLA	C1C-C2C	2.09	1.48	1.44
31	b	606	CLA	C3D-C4D	-2.09	1.39	1.44
31	C	507	CLA	C1A-CHA	2.09	1.51	1.43
31	Y	614	CLA	C1A-CHA	2.09	1.51	1.43
31	r	604	CLA	C1C-C2C	2.09	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	408	PHO	CMC-C2C	-2.09	1.46	1.51
32	a	409	PHO	CMD-C2D	-2.09	1.46	1.51
31	s1	613	CLA	C1B-NB	2.09	1.37	1.35
40	c1	519	DGD	CGB-CFB	-2.09	1.32	1.49
31	R	604	CLA	C1A-CHA	2.08	1.51	1.43
40	b1	623	DGD	O5D-C1E	2.08	1.43	1.40
31	B	608	CLA	C1C-C2C	2.08	1.48	1.44
31	C	510	CLA	C1A-CHA	2.08	1.51	1.43
31	c	502	CLA	C3D-C4D	-2.08	1.39	1.44
31	r	613	CLA	C3B-C2B	-2.08	1.37	1.40
31	s	604	CLA	C1B-NB	2.08	1.37	1.35
31	Y	604	CLA	C1A-CHA	2.08	1.51	1.43
31	b	612	CLA	C3D-C4D	-2.08	1.39	1.44
31	r1	612	CLA	C1C-C2C	2.08	1.48	1.44
31	s1	604	CLA	C1B-NB	2.08	1.37	1.35
31	C	509	CLA	C1A-CHA	2.08	1.51	1.43
47	S	608	CHL	C3B-C2B	-2.08	1.37	1.40
31	c	507	CLA	C3D-C4D	-2.08	1.39	1.44
31	C1	503	CLA	C3D-C4D	-2.08	1.39	1.44
31	y1	603	CLA	C1A-CHA	2.08	1.51	1.43
31	R1	609	CLA	C1C-C2C	2.08	1.48	1.44
31	c	511	CLA	C3D-C4D	-2.08	1.39	1.44
31	r	603	CLA	C1B-NB	2.08	1.37	1.35
31	R1	612	CLA	C1B-NB	2.08	1.37	1.35
31	Y1	604	CLA	C1C-C2C	2.08	1.48	1.44
31	y	610	CLA	C1C-C2C	2.08	1.48	1.44
31	g1	604	CLA	C1C-C2C	2.08	1.48	1.44
31	s1	609	CLA	C1C-C2C	2.08	1.48	1.44
31	C	504	CLA	C1A-CHA	2.08	1.51	1.43
31	s	612	CLA	C1A-CHA	2.08	1.51	1.43
31	c1	508	CLA	C1A-CHA	2.08	1.51	1.43
44	d	405	PL9	C46-C44	-2.08	1.47	1.51
31	N	611	CLA	MG-NC	2.08	2.11	2.06
31	Y	612	CLA	C1A-CHA	2.08	1.51	1.43
31	C	512	CLA	C1C-C2C	2.08	1.48	1.44
31	b	612	CLA	C3B-C2B	-2.08	1.37	1.40
31	Y1	613	CLA	C3D-C4D	-2.08	1.39	1.44
31	A	410	CLA	C3D-C4D	-2.08	1.39	1.44
31	B	612	CLA	C1C-C2C	2.08	1.48	1.44
31	C1	501	CLA	C3D-C4D	-2.08	1.39	1.44
31	N1	614	CLA	C1B-NB	2.08	1.37	1.35
31	B	611	CLA	C1A-CHA	2.07	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	F1	101	HEM	CAA-C2A	2.07	1.55	1.52
31	b1	602	CLA	C1B-NB	2.07	1.37	1.35
31	s	611	CLA	C1C-C2C	2.07	1.48	1.44
31	Y1	603	CLA	C1A-CHA	2.07	1.51	1.43
31	R	608	CLA	C1C-C2C	2.07	1.48	1.44
31	s1	613	CLA	MG-NC	2.07	2.11	2.06
31	G	610	CLA	C1B-NB	2.07	1.37	1.35
31	B1	615	CLA	MG-NC	2.07	2.11	2.06
31	c	501	CLA	C1A-CHA	2.07	1.51	1.43
31	B1	604	CLA	C1A-CHA	2.07	1.51	1.43
31	B	602	CLA	C1C-C2C	2.07	1.48	1.44
31	S1	612	CLA	C1A-CHA	2.07	1.51	1.43
31	S	609	CLA	C1B-NB	2.07	1.37	1.35
31	N1	610	CLA	C1A-CHA	2.07	1.51	1.43
31	A	407	CLA	C3D-C4D	-2.07	1.39	1.44
31	B1	606	CLA	C3D-C4D	-2.07	1.39	1.44
31	C	501	CLA	C1A-CHA	2.07	1.51	1.43
56	r1	626	ERG	C11-C9	2.07	1.57	1.53
32	A1	408	PHO	CMB-C2B	-2.07	1.46	1.51
31	a1	406	CLA	C1C-C2C	2.07	1.48	1.44
31	d	402	CLA	C3D-C4D	-2.07	1.39	1.44
31	c	503	CLA	C1C-C2C	2.07	1.48	1.44
31	c	505	CLA	C1C-C2C	2.07	1.48	1.44
31	g1	611	CLA	C1C-C2C	2.07	1.48	1.44
35	h1	102	LMG	C22-C21	-2.07	1.32	1.49
31	B	604	CLA	C1A-CHA	2.07	1.51	1.43
31	y1	614	CLA	C3D-C4D	-2.07	1.39	1.44
47	g	609	CHL	C3B-C2B	-2.07	1.37	1.40
31	G	602	CLA	C3B-C2B	-2.07	1.37	1.40
31	s1	617	CLA	C1B-NB	2.07	1.37	1.35
31	Y1	614	CLA	C1A-CHA	2.07	1.51	1.43
31	b1	606	CLA	C1A-CHA	2.07	1.51	1.43
31	y	610	CLA	C3B-C2B	-2.07	1.37	1.40
31	b	617	CLA	C1A-CHA	2.07	1.51	1.43
31	G1	603	CLA	C1A-CHA	2.06	1.51	1.43
31	C1	508	CLA	C1C-C2C	2.06	1.48	1.44
31	G1	610	CLA	C1A-CHA	2.06	1.51	1.43
31	B1	613	CLA	C1A-CHA	2.06	1.51	1.43
31	C	509	CLA	C3D-C4D	-2.06	1.39	1.44
31	a	410	CLA	C3D-C4D	-2.06	1.39	1.44
31	D1	402	CLA	C3D-C4D	-2.06	1.39	1.44
31	d1	402	CLA	C1A-CHA	2.06	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S1	613	CLA	C1B-NB	2.06	1.37	1.35
31	B1	604	CLA	C3D-C4D	-2.06	1.39	1.44
31	S	617	CLA	MG-NC	2.06	2.11	2.06
57	Y1	626	PTY	O7-C8	2.06	1.40	1.34
50	s	623	NEX	C16-C1	2.06	1.57	1.53
32	A	408	PHO	CMD-C2D	-2.06	1.46	1.51
44	D1	405	PL9	C3-C4	-2.06	1.46	1.49
31	N1	604	CLA	C1A-CHA	2.06	1.51	1.43
31	G1	614	CLA	C1B-NB	2.06	1.37	1.35
31	b	602	CLA	C1C-C2C	2.06	1.48	1.44
31	g1	603	CLA	MG-NC	2.06	2.11	2.06
31	b	610	CLA	C1A-CHA	2.06	1.51	1.43
47	g1	606	CHL	C3B-C2B	-2.06	1.37	1.40
31	n	613	CLA	MG-NC	2.06	2.11	2.06
31	N	613	CLA	C3B-C2B	-2.06	1.37	1.40
31	c	505	CLA	C3D-C4D	-2.06	1.39	1.44
31	R1	604	CLA	CHD-C1D	2.06	1.42	1.38
47	Y1	605	CHL	C3B-C2B	-2.06	1.37	1.40
47	n	609	CHL	C3A-C2A	-2.05	1.48	1.54
44	D1	405	PL9	C7-C3	-2.05	1.49	1.51
31	n1	602	CLA	C1A-CHA	2.05	1.51	1.43
31	N1	610	CLA	C3D-C4D	-2.05	1.39	1.44
31	R1	608	CLA	MG-NC	2.05	2.11	2.06
31	C	501	CLA	C1C-C2C	2.05	1.48	1.44
31	N1	602	CLA	C1A-CHA	2.05	1.51	1.43
31	g	604	CLA	C3B-C2B	-2.05	1.37	1.40
31	S	612	CLA	C1C-C2C	2.05	1.48	1.44
31	B1	614	CLA	C1C-C2C	2.05	1.48	1.44
31	g1	611	CLA	C1B-NB	2.05	1.37	1.35
52	b1	624	3PH	O31-C3	-2.05	1.40	1.45
31	s	610	CLA	C1C-C2C	2.05	1.48	1.44
31	D	402	CLA	C3D-C4D	-2.05	1.39	1.44
32	A	408	PHO	CMB-C2B	-2.05	1.46	1.51
31	N1	611	CLA	C1C-C2C	2.05	1.48	1.44
33	C1	516	BCR	C12-C13	-2.05	1.41	1.45
31	g	602	CLA	C1A-CHA	2.05	1.51	1.43
31	r	610	CLA	C1B-NB	2.05	1.37	1.35
31	b1	617	CLA	C1B-NB	2.05	1.37	1.35
32	A1	409	PHO	CMD-C2D	-2.05	1.46	1.51
47	G	608	CHL	C3B-C2B	-2.05	1.37	1.40
31	Y1	613	CLA	C3B-C2B	-2.05	1.37	1.40
47	S	606	CHL	C3B-C2B	-2.05	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	602	CLA	C3D-C4D	-2.05	1.39	1.44
31	s	617	CLA	MG-NC	2.05	2.11	2.06
31	N	602	CLA	C1B-NB	2.05	1.37	1.35
32	A	409	PHO	CMB-C2B	-2.05	1.46	1.51
31	B	613	CLA	C1A-CHA	2.05	1.51	1.43
31	C	508	CLA	C3D-C4D	-2.05	1.39	1.44
32	a1	408	PHO	CMD-C2D	-2.05	1.46	1.51
57	Y1	627	PTY	O4-C1	-2.05	1.40	1.45
32	A1	408	PHO	CMC-C2C	-2.05	1.46	1.51
31	c1	511	CLA	C3B-C2B	-2.05	1.37	1.40
31	S	610	CLA	C3D-C4D	-2.04	1.39	1.44
31	b	612	CLA	C1A-CHA	2.04	1.51	1.43
31	b1	609	CLA	CHD-C1D	2.04	1.42	1.38
31	S	613	CLA	C1C-C2C	2.04	1.48	1.44
31	R	603	CLA	C1B-NB	2.04	1.37	1.35
31	B	606	CLA	C3D-C4D	-2.04	1.39	1.44
31	d1	402	CLA	C3D-C4D	-2.04	1.39	1.44
31	S1	603	CLA	C1C-C2C	2.04	1.48	1.44
31	Y	603	CLA	C1A-CHA	2.04	1.51	1.43
31	c1	512	CLA	C1C-C2C	2.04	1.48	1.44
31	b1	606	CLA	C3D-C4D	-2.04	1.39	1.44
31	a1	410	CLA	C1C-C2C	2.04	1.48	1.44
31	g1	612	CLA	C1C-C2C	2.04	1.48	1.44
31	Y	610	CLA	C1B-NB	2.04	1.37	1.35
31	c	511	CLA	C1A-CHA	2.04	1.51	1.43
31	N	602	CLA	C3B-C2B	-2.04	1.37	1.40
31	y1	612	CLA	MG-NC	2.04	2.11	2.06
31	C1	506	CLA	C1C-C2C	2.04	1.48	1.44
31	n1	604	CLA	C1C-C2C	2.04	1.48	1.44
31	G	604	CLA	C3D-C4D	-2.04	1.39	1.44
31	C1	505	CLA	C3D-C4D	-2.04	1.39	1.44
31	s1	604	CLA	MG-NC	2.04	2.11	2.06
31	R1	609	CLA	C3B-C2B	-2.04	1.37	1.40
31	G1	602	CLA	C1A-CHA	2.04	1.51	1.43
31	Y	603	CLA	C1C-C2C	2.04	1.48	1.44
32	A1	408	PHO	CMD-C2D	-2.04	1.46	1.51
35	A	413	LMG	C22-C21	-2.04	1.33	1.49
31	g1	614	CLA	MG-NC	2.04	2.11	2.06
31	G1	613	CLA	C1C-C2C	2.04	1.48	1.44
31	S1	609	CLA	C1C-C2C	2.04	1.48	1.44
31	b1	614	CLA	MG-NC	2.04	2.11	2.06
31	y1	614	CLA	C1A-CHA	2.03	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	503	CLA	C1B-NB	2.03	1.37	1.35
31	G	611	CLA	C1C-C2C	2.03	1.48	1.44
31	r	608	CLA	C1C-C2C	2.03	1.48	1.44
31	C	502	CLA	C3D-C4D	-2.03	1.39	1.44
50	R	622	NEX	O24-C25	-2.03	1.43	1.46
31	Y	604	CLA	C3D-C4D	-2.03	1.39	1.44
31	R1	612	CLA	MG-NC	2.03	2.11	2.06
31	S1	605	CLA	C1C-C2C	2.03	1.48	1.44
31	C	510	CLA	C3D-C4D	-2.03	1.39	1.44
35	A	413	LMG	C43-C42	-2.03	1.33	1.49
31	y	602	CLA	C1A-CHA	2.03	1.51	1.43
31	B	615	CLA	C1C-C2C	2.03	1.48	1.44
31	G1	604	CLA	C3D-C4D	-2.03	1.39	1.44
31	y1	603	CLA	C1B-NB	2.03	1.37	1.35
44	d	405	PL9	C52-C5	-2.03	1.46	1.50
31	G1	603	CLA	C1C-C2C	2.03	1.48	1.44
31	R	604	CLA	C3B-C2B	-2.03	1.37	1.40
31	A1	410	CLA	C3B-C2B	-2.03	1.37	1.40
31	b1	610	CLA	MG-NC	2.03	2.11	2.06
31	b	604	CLA	C3D-C4D	-2.03	1.39	1.44
31	g1	610	CLA	C1B-NB	2.03	1.37	1.35
31	B1	613	CLA	C1C-C2C	2.03	1.48	1.44
47	G	601	CHL	CHC-C1C	2.03	1.40	1.35
31	B	606	CLA	C1A-CHA	2.03	1.51	1.43
31	S	605	CLA	C1C-C2C	2.03	1.48	1.44
31	C	507	CLA	C3D-C4D	-2.03	1.39	1.44
35	b1	622	LMG	C25-C24	-2.03	1.33	1.49
52	t1	101	3PH	O31-C3	-2.03	1.40	1.45
31	b1	606	CLA	C1C-C2C	2.03	1.48	1.44
31	Y1	608	CLA	C1B-NB	2.03	1.37	1.35
35	A1	413	LMG	C43-C42	-2.03	1.33	1.49
31	C1	502	CLA	C3D-C4D	-2.03	1.39	1.44
57	y1	627	PTY	O4-C1	-2.03	1.40	1.45
40	C	520	DGD	CDA-CCA	-2.03	1.33	1.49
31	N1	603	CLA	C1C-C2C	2.03	1.48	1.44
31	S1	612	CLA	C1C-C2C	2.03	1.48	1.44
31	N	611	CLA	C1B-NB	2.02	1.37	1.35
31	C	511	CLA	C3D-C4D	-2.02	1.39	1.44
31	d1	403	CLA	CHD-C1D	2.02	1.42	1.38
31	S	603	CLA	MG-NC	2.02	2.11	2.06
31	b	615	CLA	MG-NC	2.02	2.11	2.06
31	n1	603	CLA	C1C-C2C	2.02	1.48	1.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	610	CLA	C3D-C4D	-2.02	1.39	1.44
31	b	610	CLA	C3D-C4D	-2.02	1.39	1.44
35	a1	413	LMG	C43-C42	-2.02	1.33	1.49
31	s	609	CLA	C1A-CHA	2.02	1.51	1.43
31	C1	513	CLA	C3D-C4D	-2.02	1.39	1.44
31	g	613	CLA	MG-NC	2.02	2.11	2.06
31	r	613	CLA	C1B-NB	2.02	1.37	1.35
35	h	102	LMG	C22-C21	-2.02	1.33	1.49
47	s	601	CHL	CHC-C1C	2.02	1.40	1.35
31	s	609	CLA	MG-NC	2.02	2.11	2.06
35	C	521	LMG	C25-C24	-2.02	1.33	1.49
31	C	506	CLA	C3D-C4D	-2.02	1.39	1.44
31	B	604	CLA	MG-NC	2.02	2.11	2.06
35	c	521	LMG	C43-C42	-2.02	1.33	1.49
31	B1	615	CLA	C1B-NB	2.02	1.37	1.35
31	R	608	CLA	MG-NC	2.02	2.11	2.06
40	c	520	DGD	CDA-CCA	-2.02	1.33	1.49
31	y1	608	CLA	C3D-C4D	-2.02	1.39	1.44
40	C1	518	DGD	CGB-CFB	-2.02	1.33	1.49
40	C	518	DGD	CGB-CFB	-2.02	1.33	1.49
31	Y1	612	CLA	C1C-C2C	2.02	1.48	1.44
47	y	609	CHL	C3B-C2B	-2.02	1.37	1.40
31	S	611	CLA	MG-NC	2.02	2.11	2.06
31	B	616	CLA	C1C-C2C	2.02	1.48	1.44
31	Y	602	CLA	C3D-C4D	-2.02	1.39	1.44
31	r1	608	CLA	MG-NC	2.02	2.11	2.06
31	N	602	CLA	C1A-CHA	2.02	1.51	1.43
44	D1	405	PL9	C52-C5	-2.02	1.46	1.50
31	y	613	CLA	C3D-C4D	-2.02	1.39	1.44
31	C1	503	CLA	C1C-C2C	2.02	1.48	1.44
31	Y1	603	CLA	C1C-C2C	2.02	1.48	1.44
31	A1	405	CLA	C3B-C2B	-2.02	1.37	1.40
31	a1	406	CLA	C3B-C2B	-2.02	1.37	1.40
47	g	608	CHL	C3B-C2B	-2.02	1.37	1.40
31	r	612	CLA	MG-NC	2.02	2.11	2.06
31	Y	608	CLA	MG-NC	2.02	2.11	2.06
31	A	410	CLA	C1C-C2C	2.02	1.48	1.44
40	c	518	DGD	CGB-CFB	-2.02	1.33	1.49
31	B1	607	CLA	C3D-C4D	-2.02	1.39	1.44
31	c	510	CLA	C1A-CHA	2.02	1.51	1.43
31	r1	602	CLA	C3B-C2B	-2.02	1.37	1.40
35	h	102	LMG	C43-C42	-2.02	1.33	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n1	603	CLA	C1B-NB	2.02	1.37	1.35
31	c1	505	CLA	MG-NC	2.01	2.11	2.06
31	c1	507	CLA	C3D-C4D	-2.01	1.39	1.44
31	b	609	CLA	C1C-C2C	2.01	1.48	1.44
31	c	508	CLA	C3B-C2B	-2.01	1.37	1.40
47	n1	605	CHL	C3B-C2B	-2.01	1.37	1.40
31	g1	613	CLA	C1B-NB	2.01	1.37	1.35
31	b	604	CLA	C1C-C2C	2.01	1.48	1.44
31	B	607	CLA	CHD-C1D	2.01	1.42	1.38
31	R1	603	CLA	C3D-C4D	-2.01	1.39	1.44
40	C1	520	DGD	CDA-CCA	-2.01	1.33	1.49
40	c1	519	DGD	CGA-CFA	-2.01	1.33	1.49
31	g	610	CLA	C1A-CHA	2.01	1.51	1.43
40	c	519	DGD	CGB-CFB	-2.01	1.33	1.49
31	g1	610	CLA	C3B-C2B	-2.01	1.37	1.40
31	s1	602	CLA	C3D-C4D	-2.01	1.39	1.44
31	y1	603	CLA	C1C-C2C	2.01	1.48	1.44
31	B	613	CLA	C3B-C2B	-2.01	1.37	1.40
31	Y1	602	CLA	C3D-C4D	-2.01	1.39	1.44
35	a	413	LMG	C22-C21	-2.01	1.33	1.49
35	D1	411	LMG	C25-C24	-2.01	1.33	1.49
40	C1	519	DGD	CGB-CFB	-2.01	1.33	1.49
35	b	622	LMG	C25-C24	-2.01	1.33	1.49
31	C1	507	CLA	C1A-CHA	2.01	1.51	1.43
31	n1	610	CLA	C3B-C2B	-2.01	1.37	1.40
31	C	503	CLA	C3D-C4D	-2.01	1.39	1.44
31	n1	603	CLA	MG-NC	2.01	2.11	2.06
31	B	607	CLA	C3D-C4D	-2.01	1.39	1.44
31	b1	615	CLA	CHD-C1D	2.01	1.42	1.38
35	c1	521	LMG	C43-C42	-2.01	1.33	1.49
31	S	609	CLA	MG-NC	2.01	2.11	2.06
35	C1	521	LMG	C25-C24	-2.01	1.33	1.49
40	C	520	DGD	CGB-CFB	-2.01	1.33	1.49
31	n1	611	CLA	C1B-NB	2.01	1.37	1.35
35	H	102	LMG	C43-C42	-2.01	1.33	1.49
31	S1	610	CLA	C3D-C4D	-2.01	1.39	1.44
31	r	602	CLA	MG-NC	2.01	2.11	2.06
31	r	611	CLA	MG-NC	2.01	2.11	2.06
31	b	611	CLA	C3D-C4D	-2.01	1.39	1.44
31	c	506	CLA	C3D-C4D	-2.01	1.39	1.44
35	a1	413	LMG	C22-C21	-2.01	1.33	1.49
31	R	611	CLA	MG-NC	2.01	2.11	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r1	602	CLA	C1B-NB	2.01	1.37	1.35
31	S1	605	CLA	C3D-C4D	-2.01	1.39	1.44
31	s1	603	CLA	MG-NC	2.01	2.11	2.06
35	D	411	LMG	C25-C24	-2.01	1.33	1.49
40	c1	518	DGD	CGB-CFB	-2.01	1.33	1.49
31	N	603	CLA	C3D-C4D	-2.01	1.39	1.44
31	Y	603	CLA	C3D-C4D	-2.01	1.39	1.44
31	s	603	CLA	MG-NC	2.01	2.11	2.06
47	n	601	CHL	C3B-C2B	-2.00	1.37	1.40
31	B	605	CLA	C3D-C4D	-2.00	1.39	1.44
35	C	521	LMG	C43-C42	-2.00	1.33	1.49
40	C	519	DGD	CGB-CFB	-2.00	1.33	1.49
31	a	405	CLA	C3D-C4D	-2.00	1.39	1.44
31	G	613	CLA	MG-NC	2.00	2.11	2.06
40	C1	520	DGD	CGB-CFB	-2.00	1.33	1.49
35	B1	622	LMG	C25-C24	-2.00	1.33	1.49
52	T1	101	3PH	O21-C2	-2.00	1.41	1.46
31	N1	613	CLA	MG-NC	2.00	2.11	2.06
31	C1	507	CLA	C3D-C4D	-2.00	1.39	1.44
35	A1	413	LMG	C22-C21	-2.00	1.33	1.49
31	s1	609	CLA	MG-NC	2.00	2.11	2.06
31	B1	603	CLA	C1C-C2C	2.00	1.48	1.44
31	R1	602	CLA	C1C-C2C	2.00	1.48	1.44
31	C	504	CLA	C3D-C4D	-2.00	1.39	1.44
31	c	508	CLA	C3D-C4D	-2.00	1.39	1.44
35	a	413	LMG	C43-C42	-2.00	1.33	1.49
31	S	603	CLA	C1B-NB	2.00	1.37	1.35
35	H	102	LMG	C22-C21	-2.00	1.33	1.49
31	b1	604	CLA	C1C-C2C	2.00	1.48	1.44
50	g	623	NEX	O24-C25	-2.00	1.43	1.46
31	b	602	CLA	C3D-C4D	-2.00	1.39	1.44
31	b1	617	CLA	C3D-C4D	-2.00	1.39	1.44
31	b1	610	CLA	C1B-NB	2.00	1.37	1.35
31	G1	612	CLA	MG-NC	2.00	2.11	2.06
35	H1	102	LMG	C43-C42	-2.00	1.33	1.49
35	c1	521	LMG	C25-C24	-2.00	1.33	1.49
47	S1	607	CHL	C3B-C2B	-2.00	1.37	1.40
40	C1	519	DGD	CGA-CFA	-2.00	1.33	1.49
31	A	407	CLA	CHD-C1D	2.00	1.42	1.38

All (8419) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H	101	RRX	C37-C22-C23	-30.79	69.57	118.08
41	L1	101	LHG	O7-C7-C8	23.38	161.90	111.50
31	R1	609	CLA	C4-C3-C5	-22.81	76.90	115.27
52	S1	626	3PH	O21-C21-C22	22.50	160.00	111.50
31	B	617	CLA	C4-C3-C5	-22.49	77.43	115.27
52	s1	626	3PH	O21-C21-C22	22.41	159.81	111.50
31	b	617	CLA	C4-C3-C5	-22.17	77.98	115.27
46	H	101	RRX	C20-C21-C22	20.08	155.97	127.31
31	b	617	CLA	C5-C3-C2	18.94	159.44	121.12
31	B	617	CLA	C5-C3-C2	18.90	159.35	121.12
31	R1	609	CLA	C5-C3-C2	18.69	158.93	121.12
46	H	101	RRX	C37-C22-C21	18.42	148.72	122.92
52	s1	626	3PH	O21-C21-O22	-18.19	79.75	123.70
52	S1	626	3PH	O21-C21-O22	-18.17	79.80	123.70
41	L1	101	LHG	O7-C7-O9	-17.96	80.30	123.70
33	c1	514	BCR	C10-C11-C12	17.89	179.03	123.22
33	C1	517	BCR	C10-C11-C12	17.76	178.63	123.22
33	B1	618	BCR	C10-C11-C12	17.71	178.49	123.22
33	C	517	BCR	C10-C11-C12	17.70	178.45	123.22
33	C1	514	BCR	C10-C11-C12	17.68	178.38	123.22
33	b1	618	BCR	C10-C11-C12	17.45	177.66	123.22
33	c	514	BCR	C10-C11-C12	17.41	177.54	123.22
33	b	619	BCR	C10-C11-C12	17.40	177.53	123.22
33	D	404	BCR	C10-C11-C12	17.39	177.50	123.22
33	c1	516	BCR	C10-C11-C12	17.38	177.47	123.22
33	B	619	BCR	C10-C11-C12	17.38	177.45	123.22
33	B1	619	BCR	C10-C11-C12	17.33	177.31	123.22
33	C	516	BCR	C10-C11-C12	17.33	177.30	123.22
33	b1	619	BCR	C10-C11-C12	17.32	177.28	123.22
33	B	618	BCR	C10-C11-C12	17.30	177.20	123.22
33	c	515	BCR	C10-C11-C12	17.30	177.20	123.22
33	C1	515	BCR	C10-C11-C12	17.29	177.19	123.22
49	Y1	622	XAT	C37-C21-C36	-17.26	81.91	107.37
33	a1	411	BCR	C10-C11-C12	17.22	176.96	123.22
33	b	618	BCR	C10-C11-C12	17.22	176.96	123.22
33	C	515	BCR	C10-C11-C12	17.15	176.75	123.22
33	c1	515	BCR	C10-C11-C12	17.15	176.74	123.22
33	a	411	BCR	C10-C11-C12	17.14	176.71	123.22
33	C	514	BCR	C10-C11-C12	17.09	176.54	123.22
49	Y	622	XAT	C37-C21-C36	-17.07	82.19	107.37
33	c	517	BCR	C10-C11-C12	17.05	176.43	123.22
33	d	404	BCR	C10-C11-C12	16.94	176.07	123.22
33	c	516	BCR	C10-C11-C12	16.87	175.87	123.22

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	y	622	XAT	C37-C21-C36	-16.86	82.50	107.37
49	y1	622	XAT	C37-C21-C36	-16.83	82.55	107.37
33	A	411	BCR	C10-C11-C12	16.80	175.65	123.22
33	A1	411	BCR	C10-C11-C12	16.80	175.64	123.22
33	D1	404	BCR	C10-C11-C12	16.68	175.27	123.22
33	d1	404	BCR	C10-C11-C12	16.56	174.91	123.22
31	b	617	CLA	C4-C3-C2	-16.45	81.47	123.68
31	B	617	CLA	C4-C3-C2	-16.26	81.96	123.68
31	R1	609	CLA	C4-C3-C2	-16.23	82.04	123.68
33	c1	517	BCR	C10-C11-C12	16.04	173.26	123.22
33	C1	516	BCR	C10-C11-C12	15.94	172.97	123.22
33	B1	618	BCR	C16-C15-C14	14.91	154.02	123.47
33	c1	514	BCR	C16-C15-C14	14.89	153.98	123.47
33	c	514	BCR	C16-C15-C14	14.89	153.97	123.47
46	H	101	RRX	C23-C22-C21	14.81	141.66	118.94
33	b1	618	BCR	C16-C15-C14	14.78	153.76	123.47
33	c1	517	BCR	C16-C15-C14	14.69	153.56	123.47
33	C	514	BCR	C16-C15-C14	14.63	153.44	123.47
33	C1	517	BCR	C16-C15-C14	14.29	152.74	123.47
33	C1	514	BCR	C16-C15-C14	14.28	152.73	123.47
33	a1	411	BCR	C11-C10-C9	14.24	147.64	127.31
33	c1	517	BCR	C11-C10-C9	14.16	147.52	127.31
33	B1	619	BCR	C16-C15-C14	14.06	152.28	123.47
33	A1	411	BCR	C11-C10-C9	14.06	147.37	127.31
33	b	619	BCR	C16-C15-C14	13.97	152.09	123.47
33	B	618	BCR	C16-C15-C14	13.89	151.93	123.47
33	c1	517	BCR	C21-C20-C19	13.76	166.17	123.22
33	A1	411	BCR	C21-C20-C19	13.71	166.00	123.22
33	C	516	BCR	C11-C10-C9	13.70	146.86	127.31
33	C1	515	BCR	C16-C15-C14	13.67	151.47	123.47
33	C1	516	BCR	C11-C10-C9	13.64	146.78	127.31
33	c1	516	BCR	C11-C10-C9	13.64	146.78	127.31
56	r1	626	ERG	C15-C14-C8	-13.63	99.78	120.44
33	b	618	BCR	C11-C10-C9	13.62	146.75	127.31
33	b1	619	BCR	C16-C15-C14	13.58	151.29	123.47
33	C	514	BCR	C11-C10-C9	13.57	146.67	127.31
33	C1	517	BCR	C21-C20-C19	13.56	165.54	123.22
33	D1	404	BCR	C21-C20-C19	13.50	165.35	123.22
33	B	619	BCR	C21-C20-C19	13.47	165.26	123.22
33	A	411	BCR	C11-C10-C9	13.40	146.43	127.31
33	c	514	BCR	C11-C10-C9	13.34	146.35	127.31
33	C1	515	BCR	C11-C10-C9	13.21	146.16	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	618	BCR	C11-C10-C9	13.15	146.07	127.31
33	a1	411	BCR	C16-C15-C14	13.12	150.35	123.47
33	C1	517	BCR	C11-C10-C9	13.03	145.91	127.31
33	C1	514	BCR	C11-C10-C9	12.99	145.85	127.31
33	C1	516	BCR	C16-C15-C14	12.94	149.98	123.47
33	c	517	BCR	C16-C15-C14	12.93	149.95	123.47
33	c	517	BCR	C11-C10-C9	12.90	145.72	127.31
33	D1	404	BCR	C16-C15-C14	12.90	149.90	123.47
33	C	517	BCR	C21-C20-C19	12.87	163.38	123.22
33	c1	516	BCR	C16-C15-C14	12.85	149.79	123.47
33	a	411	BCR	C21-C20-C19	12.81	163.20	123.22
33	b	619	BCR	C11-C10-C9	12.81	145.60	127.31
33	c	517	BCR	C21-C20-C19	12.79	163.15	123.22
33	D	404	BCR	C11-C10-C9	12.77	145.54	127.31
33	b	619	BCR	C21-C20-C19	12.71	162.87	123.22
33	C1	516	BCR	C21-C20-C19	12.68	162.77	123.22
33	C	515	BCR	C16-C15-C14	12.67	149.43	123.47
33	C	517	BCR	C16-C15-C14	12.66	149.40	123.47
33	b	618	BCR	C16-C15-C14	12.61	149.30	123.47
33	c	516	BCR	C16-C15-C14	12.60	149.28	123.47
33	a	411	BCR	C11-C10-C9	12.60	145.29	127.31
33	c1	515	BCR	C16-C15-C14	12.59	149.25	123.47
33	A1	411	BCR	C16-C15-C14	12.56	149.21	123.47
33	b1	618	BCR	C11-C10-C9	12.53	145.20	127.31
33	c	516	BCR	C11-C10-C9	12.51	145.16	127.31
33	c1	516	BCR	C21-C20-C19	12.49	162.20	123.22
33	B1	618	BCR	C11-C10-C9	12.49	145.14	127.31
49	y	622	XAT	C37-C21-C22	-12.48	87.29	108.98
33	c1	515	BCR	C11-C10-C9	12.42	145.03	127.31
33	B1	619	BCR	C11-C10-C9	12.39	144.99	127.31
33	c	515	BCR	C16-C15-C14	12.37	148.82	123.47
49	Y	622	XAT	C37-C21-C22	-12.35	87.53	108.98
33	b1	619	BCR	C21-C20-C19	12.32	161.67	123.22
33	A	411	BCR	C16-C15-C14	12.29	148.65	123.47
33	a	411	BCR	C16-C15-C14	12.26	148.60	123.47
33	C	514	BCR	C21-C20-C19	12.26	161.49	123.22
49	Y1	622	XAT	C37-C21-C22	-12.25	87.70	108.98
33	a1	411	BCR	C21-C20-C19	12.21	161.32	123.22
33	C	516	BCR	C16-C15-C14	12.18	148.42	123.47
33	b1	619	BCR	C11-C10-C9	12.18	144.69	127.31
33	c1	514	BCR	C11-C10-C9	12.16	144.67	127.31
33	C	515	BCR	C11-C10-C9	12.15	144.65	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	y1	622	XAT	C37-C21-C22	-12.10	87.96	108.98
33	B1	618	BCR	C21-C20-C19	12.09	160.96	123.22
33	c	514	BCR	C21-C20-C19	12.07	160.90	123.22
33	B	619	BCR	C16-C15-C14	12.03	148.13	123.47
33	c	515	BCR	C11-C10-C9	12.01	144.45	127.31
33	B1	619	BCR	C21-C20-C19	11.97	160.57	123.22
33	d1	404	BCR	C21-C20-C19	11.93	160.46	123.22
33	D	404	BCR	C16-C15-C14	11.79	147.63	123.47
33	d1	404	BCR	C16-C15-C14	11.78	147.60	123.47
33	A	411	BCR	C21-C20-C19	11.75	159.89	123.22
33	b	618	BCR	C21-C20-C19	11.70	159.73	123.22
33	c1	514	BCR	C21-C20-C19	11.69	159.69	123.22
33	d	404	BCR	C16-C15-C14	11.66	147.35	123.47
33	b1	618	BCR	C21-C20-C19	11.56	159.30	123.22
33	C1	514	BCR	C21-C20-C19	11.52	159.16	123.22
33	d1	404	BCR	C11-C10-C9	11.45	143.65	127.31
31	b1	605	CLA	C4A-NA-C1A	11.40	111.83	106.71
33	B	619	BCR	C11-C10-C9	11.36	143.52	127.31
33	C	515	BCR	C11-C12-C13	11.33	158.26	126.42
33	B	618	BCR	C21-C20-C19	11.31	158.51	123.22
33	C	517	BCR	C11-C10-C9	11.31	143.45	127.31
52	s1	626	3PH	O22-C21-C22	-11.19	80.08	123.73
33	d	404	BCR	C11-C10-C9	11.18	143.26	127.31
52	S1	626	3PH	O22-C21-C22	-11.16	80.20	123.73
33	C	515	BCR	C21-C20-C19	11.13	157.94	123.22
33	D	404	BCR	C11-C12-C13	11.13	157.67	126.42
33	a	411	BCR	C11-C12-C13	11.05	157.46	126.42
33	B	619	BCR	C11-C12-C13	11.05	157.45	126.42
33	c1	515	BCR	C11-C12-C13	10.98	157.26	126.42
33	d	404	BCR	C11-C12-C13	10.98	157.25	126.42
33	c1	515	BCR	C21-C20-C19	10.96	157.43	123.22
33	a1	411	BCR	C11-C12-C13	10.91	157.08	126.42
33	B1	619	BCR	C11-C12-C13	10.85	156.91	126.42
33	C1	517	BCR	C11-C12-C13	10.83	156.84	126.42
33	C	516	BCR	C11-C12-C13	10.74	156.58	126.42
33	d1	404	BCR	C11-C12-C13	10.73	156.56	126.42
31	n	604	CLA	C4A-NA-C1A	10.71	111.52	106.71
33	A1	411	BCR	C11-C12-C13	10.71	156.49	126.42
41	L1	101	LHG	O9-C7-C8	-10.70	82.00	123.73
33	c	516	BCR	C21-C20-C19	10.60	156.31	123.22
31	b	605	CLA	C4A-NA-C1A	10.57	111.46	106.71
56	R1	626	ERG	C15-C14-C8	-10.52	104.50	120.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	517	BCR	C11-C12-C13	10.49	155.88	126.42
33	c1	516	BCR	C11-C12-C13	10.49	155.88	126.42
33	c	515	BCR	C11-C12-C13	10.49	155.88	126.42
33	b1	619	BCR	C11-C12-C13	10.49	155.87	126.42
33	b	618	BCR	C11-C12-C13	10.40	155.65	126.42
33	B	618	BCR	C11-C12-C13	10.37	155.55	126.42
31	b1	612	CLA	C4A-NA-C1A	10.26	111.32	106.71
33	C	517	BCR	C11-C12-C13	10.24	155.19	126.42
33	C1	515	BCR	C21-C20-C19	10.23	155.14	123.22
33	A	411	BCR	C11-C12-C13	10.22	155.12	126.42
31	B	605	CLA	C4A-NA-C1A	10.15	111.27	106.71
33	D1	404	BCR	C11-C10-C9	10.15	141.79	127.31
33	c	516	BCR	C11-C12-C13	10.14	154.90	126.42
31	S	613	CLA	C4A-NA-C1A	10.11	111.25	106.71
31	B1	605	CLA	C4A-NA-C1A	10.11	111.25	106.71
33	c	515	BCR	C21-C20-C19	10.06	154.61	123.22
33	b	619	BCR	C11-C12-C13	10.03	154.60	126.42
33	C1	514	BCR	C11-C12-C13	10.00	154.51	126.42
31	Y1	610	CLA	C4A-NA-C1A	9.99	111.20	106.71
33	C	516	BCR	C20-C19-C18	9.97	154.43	126.42
33	C1	515	BCR	C11-C12-C13	9.97	154.42	126.42
31	a1	406	CLA	C4A-NA-C1A	9.94	111.18	106.71
31	b	606	CLA	C4A-NA-C1A	9.94	111.18	106.71
31	a1	405	CLA	C4A-NA-C1A	9.91	111.16	106.71
31	c1	502	CLA	C4A-NA-C1A	9.90	111.16	106.71
31	a	406	CLA	C4A-NA-C1A	9.89	111.15	106.71
31	b	615	CLA	C4A-NA-C1A	9.86	111.14	106.71
31	C	505	CLA	C4A-NA-C1A	9.81	111.11	106.71
31	C1	513	CLA	C4A-NA-C1A	9.80	111.11	106.71
31	C1	509	CLA	C4A-NA-C1A	9.79	111.11	106.71
31	A1	410	CLA	C4A-NA-C1A	9.77	111.10	106.71
31	c1	511	CLA	C4A-NA-C1A	9.77	111.10	106.71
31	s	602	CLA	C4A-NA-C1A	9.76	111.10	106.71
31	G1	602	CLA	C4A-NA-C1A	9.74	111.09	106.71
33	b1	618	BCR	C11-C12-C13	9.74	153.77	126.42
31	Y	610	CLA	C4A-NA-C1A	9.73	111.08	106.71
31	b1	610	CLA	C4A-NA-C1A	9.72	111.08	106.71
31	B	615	CLA	C4A-NA-C1A	9.72	111.07	106.71
31	G	603	CLA	C4A-NA-C1A	9.69	111.06	106.71
31	A	406	CLA	C4A-NA-C1A	9.67	111.06	106.71
33	d	404	BCR	C21-C20-C19	9.66	153.36	123.22
31	n	603	CLA	C4A-NA-C1A	9.66	111.05	106.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	603	CLA	C4A-NA-C1A	9.65	111.04	106.71
31	N1	603	CLA	C4A-NA-C1A	9.64	111.04	106.71
31	a	405	CLA	C4A-NA-C1A	9.60	111.02	106.71
33	C1	515	BCR	C20-C19-C18	9.59	153.37	126.42
31	s	613	CLA	C4A-NA-C1A	9.59	111.02	106.71
31	y	602	CLA	C4A-NA-C1A	9.58	111.01	106.71
31	n1	613	CLA	C4A-NA-C1A	9.58	111.01	106.71
31	b	617	CLA	C4A-NA-C1A	9.57	111.01	106.71
33	B1	618	BCR	C11-C12-C13	9.55	153.24	126.42
31	c	508	CLA	C4A-NA-C1A	9.54	111.00	106.71
33	C	516	BCR	C21-C20-C19	9.54	152.98	123.22
31	S1	612	CLA	C4A-NA-C1A	9.53	110.99	106.71
31	g1	613	CLA	C4A-NA-C1A	9.53	110.99	106.71
31	C	513	CLA	C4A-NA-C1A	9.52	110.98	106.71
31	s1	603	CLA	C4A-NA-C1A	9.51	110.98	106.71
31	C1	511	CLA	C4A-NA-C1A	9.51	110.98	106.71
31	B	613	CLA	C4A-NA-C1A	9.51	110.98	106.71
31	C1	504	CLA	C4A-NA-C1A	9.50	110.98	106.71
31	G	610	CLA	C4A-NA-C1A	9.49	110.97	106.71
31	Y	613	CLA	C4A-NA-C1A	9.49	110.97	106.71
31	g	603	CLA	C4A-NA-C1A	9.49	110.97	106.71
31	y1	613	CLA	C4A-NA-C1A	9.48	110.97	106.71
31	c	502	CLA	C4A-NA-C1A	9.48	110.97	106.71
31	r1	604	CLA	C4A-NA-C1A	9.47	110.96	106.71
33	C	514	BCR	C11-C12-C13	9.46	152.98	126.42
31	c	505	CLA	C4A-NA-C1A	9.46	110.96	106.71
31	c1	504	CLA	C4A-NA-C1A	9.45	110.95	106.71
31	c1	503	CLA	C4A-NA-C1A	9.44	110.95	106.71
31	N1	614	CLA	C4A-NA-C1A	9.43	110.95	106.71
31	R1	602	CLA	C4A-NA-C1A	9.43	110.94	106.71
31	B1	615	CLA	C4A-NA-C1A	9.42	110.94	106.71
31	n	613	CLA	C4A-NA-C1A	9.42	110.94	106.71
31	c	504	CLA	C4A-NA-C1A	9.39	110.93	106.71
31	y1	603	CLA	C4A-NA-C1A	9.38	110.92	106.71
31	b1	617	CLA	C4A-NA-C1A	9.38	110.92	106.71
31	C	511	CLA	C4A-NA-C1A	9.37	110.92	106.71
31	N1	610	CLA	C4A-NA-C1A	9.36	110.92	106.71
31	S	602	CLA	C4A-NA-C1A	9.36	110.91	106.71
31	Y1	603	CLA	C4A-NA-C1A	9.36	110.91	106.71
31	B	610	CLA	C4A-NA-C1A	9.35	110.91	106.71
31	c	507	CLA	C4A-NA-C1A	9.35	110.91	106.71
31	N1	602	CLA	C4A-NA-C1A	9.35	110.91	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	613	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	C1	505	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	S1	604	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	b1	603	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	c1	509	CLA	C4A-NA-C1A	9.34	110.91	106.71
31	N	603	CLA	C4A-NA-C1A	9.33	110.90	106.71
31	G1	610	CLA	C4A-NA-C1A	9.33	110.90	106.71
33	c	514	BCR	C11-C12-C13	9.32	152.61	126.42
33	c1	517	BCR	C11-C12-C13	9.32	152.61	126.42
31	S	605	CLA	C4A-NA-C1A	9.32	110.89	106.71
31	n	610	CLA	C4A-NA-C1A	9.32	110.89	106.71
31	b	608	CLA	C4A-NA-C1A	9.31	110.89	106.71
31	S1	613	CLA	C4A-NA-C1A	9.31	110.89	106.71
31	b	607	CLA	C4A-NA-C1A	9.30	110.89	106.71
31	b1	604	CLA	C4A-NA-C1A	9.30	110.89	106.71
31	C	504	CLA	C4A-NA-C1A	9.30	110.89	106.71
31	y	612	CLA	C4A-NA-C1A	9.30	110.89	106.71
31	b1	613	CLA	C4A-NA-C1A	9.30	110.89	106.71
31	C1	502	CLA	C4A-NA-C1A	9.29	110.88	106.71
31	y	613	CLA	C4A-NA-C1A	9.28	110.88	106.71
31	B1	613	CLA	C4A-NA-C1A	9.28	110.88	106.71
31	S1	609	CLA	C4A-NA-C1A	9.28	110.88	106.71
31	B1	603	CLA	C4A-NA-C1A	9.27	110.87	106.71
31	C1	508	CLA	C4A-NA-C1A	9.27	110.87	106.71
31	g	611	CLA	C4A-NA-C1A	9.26	110.87	106.71
31	Y1	613	CLA	C4A-NA-C1A	9.26	110.87	106.71
31	S1	611	CLA	C4A-NA-C1A	9.25	110.86	106.71
31	c1	508	CLA	C4A-NA-C1A	9.25	110.86	106.71
31	B1	606	CLA	C4A-NA-C1A	9.24	110.86	106.71
31	c1	512	CLA	C4A-NA-C1A	9.24	110.86	106.71
31	s1	612	CLA	C4A-NA-C1A	9.24	110.86	106.71
31	C	502	CLA	C4A-NA-C1A	9.23	110.86	106.71
33	D1	404	BCR	C11-C12-C13	9.22	152.32	126.42
31	A1	407	CLA	C4A-NA-C1A	9.22	110.85	106.71
31	s1	614	CLA	C4A-NA-C1A	9.22	110.85	106.71
31	B1	602	CLA	C4A-NA-C1A	9.22	110.85	106.71
31	S1	603	CLA	C4A-NA-C1A	9.22	110.85	106.71
31	b	610	CLA	C4A-NA-C1A	9.21	110.85	106.71
31	G1	613	CLA	C4A-NA-C1A	9.21	110.85	106.71
31	n1	610	CLA	C4A-NA-C1A	9.21	110.85	106.71
31	A1	406	CLA	C4A-NA-C1A	9.21	110.85	106.71
31	S	612	CLA	C4A-NA-C1A	9.20	110.84	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	512	CLA	C4A-NA-C1A	9.19	110.84	106.71
31	G1	612	CLA	C4A-NA-C1A	9.19	110.84	106.71
31	N	613	CLA	C4A-NA-C1A	9.19	110.84	106.71
31	r	613	CLA	C4A-NA-C1A	9.18	110.83	106.71
31	s1	613	CLA	C4A-NA-C1A	9.18	110.83	106.71
31	r1	602	CLA	C4A-NA-C1A	9.17	110.83	106.71
31	c	503	CLA	C4A-NA-C1A	9.17	110.83	106.71
33	c1	514	BCR	C11-C12-C13	9.17	152.16	126.42
31	B1	608	CLA	C4A-NA-C1A	9.16	110.82	106.71
31	R1	604	CLA	C4A-NA-C1A	9.16	110.82	106.71
31	R1	608	CLA	C4A-NA-C1A	9.15	110.82	106.71
31	b1	607	CLA	C4A-NA-C1A	9.15	110.82	106.71
31	R	603	CLA	C4A-NA-C1A	9.15	110.82	106.71
31	G1	614	CLA	C4A-NA-C1A	9.15	110.82	106.71
31	S1	605	CLA	C4A-NA-C1A	9.15	110.82	106.71
31	Y1	612	CLA	C4A-NA-C1A	9.14	110.81	106.71
31	G	602	CLA	C4A-NA-C1A	9.14	110.81	106.71
33	D	404	BCR	C21-C20-C19	9.13	151.72	123.22
31	B1	610	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	B	614	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	S	604	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	s1	617	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	D	402	CLA	C4A-NA-C1A	9.12	110.81	106.71
31	S1	617	CLA	C4A-NA-C1A	9.12	110.81	106.71
31	b1	602	CLA	C4A-NA-C1A	9.12	110.81	106.71
31	A	405	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	G	613	CLA	C4A-NA-C1A	9.10	110.80	106.71
31	B1	614	CLA	C4A-NA-C1A	9.10	110.80	106.71
31	s1	609	CLA	C4A-NA-C1A	9.10	110.80	106.71
31	b1	606	CLA	C4A-NA-C1A	9.10	110.80	106.71
31	s	612	CLA	C4A-NA-C1A	9.09	110.79	106.71
31	b	613	CLA	C4A-NA-C1A	9.09	110.79	106.71
31	N1	604	CLA	C4A-NA-C1A	9.09	110.79	106.71
31	g1	602	CLA	C4A-NA-C1A	9.07	110.78	106.71
31	n1	611	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	N	611	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	R	608	CLA	C4A-NA-C1A	9.05	110.78	106.71
31	r	604	CLA	C4A-NA-C1A	9.05	110.78	106.71
31	R	613	CLA	C4A-NA-C1A	9.05	110.78	106.71
31	Y	603	CLA	C4A-NA-C1A	9.05	110.77	106.71
31	y1	608	CLA	C4A-NA-C1A	9.05	110.77	106.71
31	n1	603	CLA	C4A-NA-C1A	9.04	110.77	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	501	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	S1	610	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	A	410	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	B	602	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	r	609	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	G	612	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	a	410	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	S1	602	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	b	604	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	Y	604	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	N1	612	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	B	603	CLA	C4A-NA-C1A	9.01	110.76	106.71
31	g	612	CLA	C4A-NA-C1A	9.00	110.75	106.71
31	C	510	CLA	C4A-NA-C1A	9.00	110.75	106.71
31	Y1	604	CLA	C4A-NA-C1A	8.99	110.75	106.71
31	r	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
31	s	604	CLA	C4A-NA-C1A	8.99	110.75	106.71
31	g	610	CLA	C4A-NA-C1A	8.97	110.74	106.71
31	N	614	CLA	C4A-NA-C1A	8.97	110.74	106.71
31	y	604	CLA	C4A-NA-C1A	8.96	110.74	106.71
31	b1	608	CLA	C4A-NA-C1A	8.96	110.73	106.71
31	c	506	CLA	C4A-NA-C1A	8.96	110.73	106.71
31	n1	602	CLA	C4A-NA-C1A	8.96	110.73	106.71
31	b	602	CLA	C4A-NA-C1A	8.96	110.73	106.71
31	s	614	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	R	611	CLA	C4A-NA-C1A	8.94	110.73	106.71
31	B1	611	CLA	C4A-NA-C1A	8.94	110.72	106.71
31	R1	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	g	604	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	D	403	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	r	610	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	r1	609	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	C1	506	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	N1	613	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	s1	605	CLA	C4A-NA-C1A	8.91	110.71	106.71
33	C1	516	BCR	C11-C12-C13	8.91	151.44	126.42
31	s	605	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	B1	617	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	s1	604	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	g	602	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	c	509	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	Y	614	CLA	C4A-NA-C1A	8.90	110.71	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	509	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	g1	611	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	c1	501	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	a1	407	CLA	C4A-NA-C1A	8.87	110.70	106.71
31	g1	614	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	r	602	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	C1	503	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	s1	610	CLA	C4A-NA-C1A	8.86	110.69	106.71
31	b	603	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	B	612	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	b	612	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	G	604	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	n	611	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	y1	610	CLA	C4A-NA-C1A	8.85	110.68	106.71
31	S	617	CLA	C4A-NA-C1A	8.85	110.68	106.71
31	B	608	CLA	C4A-NA-C1A	8.84	110.68	106.71
31	N	612	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	c	501	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	B	609	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	g	614	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	n1	614	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	B1	609	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	G	614	CLA	C4A-NA-C1A	8.81	110.67	106.71
33	c	515	BCR	C20-C19-C18	8.80	151.15	126.42
31	r1	608	CLA	C4A-NA-C1A	8.80	110.66	106.71
31	g1	610	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	R1	610	CLA	C4A-NA-C1A	8.79	110.66	106.71
33	c1	515	BCR	C20-C19-C18	8.78	151.09	126.42
31	C1	501	CLA	C4A-NA-C1A	8.78	110.65	106.71
31	c1	513	CLA	C4A-NA-C1A	8.76	110.65	106.71
31	R	604	CLA	C4A-NA-C1A	8.76	110.64	106.71
31	n	614	CLA	C4A-NA-C1A	8.76	110.64	106.71
31	D1	402	CLA	C4A-NA-C1A	8.76	110.64	106.71
31	N	604	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	C1	507	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	c	512	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	R	610	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	B	616	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	N	602	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	G	611	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	g1	612	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	S	611	CLA	C4A-NA-C1A	8.74	110.63	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	510	CLA	C4A-NA-C1A	8.74	110.63	106.71
31	Y	612	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	s	617	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	b1	614	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	r	611	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	R1	609	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	y1	602	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	y	614	CLA	C4A-NA-C1A	8.71	110.62	106.71
31	g1	603	CLA	C4A-NA-C1A	8.70	110.62	106.71
31	y1	611	CLA	C4A-NA-C1A	8.70	110.62	106.71
31	G1	603	CLA	C4A-NA-C1A	8.70	110.62	106.71
31	y	610	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	C	503	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	S	614	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	c1	510	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	n1	604	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	d1	403	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	y1	612	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	a1	410	CLA	C4A-NA-C1A	8.65	110.60	106.71
31	c1	506	CLA	C4A-NA-C1A	8.65	110.59	106.71
31	C	508	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	S	610	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	r	608	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	b	614	CLA	C4A-NA-C1A	8.63	110.59	106.71
31	b	616	CLA	C4A-NA-C1A	8.63	110.59	106.71
31	y	611	CLA	C4A-NA-C1A	8.63	110.59	106.71
31	Y	608	CLA	C4A-NA-C1A	8.63	110.58	106.71
31	c	513	CLA	C4A-NA-C1A	8.63	110.58	106.71
31	G1	611	CLA	C4A-NA-C1A	8.62	110.58	106.71
33	b1	618	BCR	C20-C19-C18	8.62	150.63	126.42
31	g1	604	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	B	617	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	c	510	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	y1	604	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	s	603	CLA	C4A-NA-C1A	8.60	110.57	106.71
31	c	511	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	Y1	608	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	A	407	CLA	C4A-NA-C1A	8.57	110.56	106.71
31	B1	607	CLA	C4A-NA-C1A	8.55	110.55	106.71
31	s	611	CLA	C4A-NA-C1A	8.54	110.55	106.71
31	Y1	611	CLA	C4A-NA-C1A	8.53	110.54	106.71
31	C	506	CLA	C4A-NA-C1A	8.52	110.54	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	507	CLA	C4A-NA-C1A	8.52	110.54	106.71
33	B	618	BCR	C20-C19-C18	8.52	150.35	126.42
31	C	512	CLA	C4A-NA-C1A	8.51	110.53	106.71
33	C	515	BCR	C20-C19-C18	8.49	150.26	126.42
31	r1	610	CLA	C4A-NA-C1A	8.49	110.52	106.71
31	y	608	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	R	612	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	B	606	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	S	603	CLA	C4A-NA-C1A	8.47	110.51	106.71
31	R	602	CLA	C4A-NA-C1A	8.46	110.51	106.71
31	Y	611	CLA	C4A-NA-C1A	8.43	110.50	106.71
31	b	611	CLA	C4A-NA-C1A	8.43	110.50	106.71
31	b1	611	CLA	C4A-NA-C1A	8.43	110.50	106.71
31	B	611	CLA	C4A-NA-C1A	8.42	110.49	106.71
31	S	609	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	R1	603	CLA	C4A-NA-C1A	8.40	110.48	106.71
31	b1	615	CLA	C4A-NA-C1A	8.40	110.48	106.71
31	d	403	CLA	C4A-NA-C1A	8.37	110.47	106.71
33	b	618	BCR	C20-C19-C18	8.37	149.93	126.42
46	H1	101	RRX	C38-C26-C25	-8.36	115.14	124.53
31	s	610	CLA	C4A-NA-C1A	8.36	110.47	106.71
31	B1	616	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	n1	612	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	d1	402	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	b1	616	CLA	C4A-NA-C1A	8.33	110.45	106.71
31	B1	604	CLA	C4A-NA-C1A	8.30	110.44	106.71
31	R	609	CLA	C4A-NA-C1A	8.30	110.44	106.71
31	c1	505	CLA	C4A-NA-C1A	8.30	110.44	106.71
31	s1	611	CLA	C4A-NA-C1A	8.29	110.43	106.71
31	n	602	CLA	C4A-NA-C1A	8.29	110.43	106.71
31	D1	403	CLA	C4A-NA-C1A	8.29	110.43	106.71
31	c1	507	CLA	C4A-NA-C1A	8.26	110.42	106.71
33	C1	514	BCR	C20-C19-C18	8.25	149.59	126.42
31	s	609	CLA	C4A-NA-C1A	8.25	110.41	106.71
31	S1	614	CLA	C4A-NA-C1A	8.23	110.41	106.71
31	r1	612	CLA	C4A-NA-C1A	8.23	110.41	106.71
31	a	407	CLA	C4A-NA-C1A	8.22	110.40	106.71
31	y1	614	CLA	C4A-NA-C1A	8.22	110.40	106.71
31	Y	602	CLA	C4A-NA-C1A	8.21	110.40	106.71
31	r1	603	CLA	C4A-NA-C1A	8.21	110.40	106.71
31	N	610	CLA	C4A-NA-C1A	8.21	110.39	106.71
31	N1	611	CLA	C4A-NA-C1A	8.20	110.39	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B1	612	CLA	C4A-NA-C1A	8.19	110.39	106.71
33	B1	618	BCR	C20-C19-C18	8.12	149.22	126.42
31	s1	602	CLA	C4A-NA-C1A	8.10	110.35	106.71
31	G1	604	CLA	C4A-NA-C1A	8.08	110.34	106.71
31	r	612	CLA	C4A-NA-C1A	8.07	110.33	106.71
33	B1	619	BCR	C20-C19-C18	8.00	148.88	126.42
31	B	607	CLA	C4A-NA-C1A	7.99	110.30	106.71
33	c	516	BCR	C20-C19-C18	7.97	148.81	126.42
33	A	411	BCR	C20-C19-C18	7.95	148.74	126.42
33	c	514	BCR	C20-C19-C18	7.92	148.67	126.42
31	b	609	CLA	C4A-NA-C1A	7.91	110.26	106.71
31	A1	405	CLA	C4A-NA-C1A	7.91	110.26	106.71
33	c1	514	BCR	C20-C19-C18	7.90	148.62	126.42
31	B	604	CLA	C4A-NA-C1A	7.88	110.25	106.71
33	b1	619	BCR	C20-C19-C18	7.79	148.29	126.42
31	d	402	CLA	C4A-NA-C1A	7.72	110.18	106.71
31	Y1	614	CLA	C4A-NA-C1A	7.70	110.17	106.71
42	C1	527	LMK	O2-C4-O3	-7.69	106.63	124.09
33	d1	404	BCR	C20-C19-C18	7.61	147.79	126.42
33	C1	516	BCR	C20-C19-C18	7.60	147.77	126.42
33	a1	411	BCR	C20-C19-C18	7.59	147.75	126.42
31	b1	609	CLA	C4A-NA-C1A	7.57	110.11	106.71
46	h1	101	RRX	C38-C26-C25	-7.51	116.10	124.53
33	b	619	BCR	C20-C19-C18	7.48	147.43	126.42
33	C	514	BCR	C20-C19-C18	7.39	147.19	126.42
31	Y1	602	CLA	C4A-NA-C1A	7.32	110.00	106.71
49	Y	622	XAT	C36-C21-C22	7.24	121.56	108.98
49	Y1	622	XAT	C36-C21-C22	7.23	121.55	108.98
49	y1	622	XAT	C37-C21-C26	-7.21	90.57	110.05
46	H1	101	RRX	C15-C14-C13	-7.14	117.11	127.31
33	a	411	BCR	C20-C19-C18	7.14	146.49	126.42
49	Y	622	XAT	C37-C21-C26	-7.11	90.84	110.05
49	y	622	XAT	C36-C21-C22	7.10	121.32	108.98
49	Y1	622	XAT	C37-C21-C26	-7.09	90.89	110.05
49	y	622	XAT	C37-C21-C26	-7.06	90.97	110.05
49	y1	622	XAT	C36-C21-C22	7.06	121.25	108.98
31	s	613	CLA	O2D-CGD-CBD	7.00	123.71	111.27
33	C1	517	BCR	C20-C19-C18	6.91	145.82	126.42
44	D1	405	PL9	C7-C3-C4	6.91	122.49	116.88
31	n	612	CLA	C4A-NA-C1A	6.90	109.81	106.71
50	y1	623	NEX	C17-C1-C6	-6.89	104.31	110.47
31	b1	609	CLA	O2D-CGD-CBD	6.87	123.47	111.27

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	B	625	DGA	CDB-CCB-CBB	-6.85	79.63	114.42
33	C	517	BCR	C20-C19-C18	6.85	145.65	126.42
50	Y1	623	NEX	C16-C1-C6	-6.83	104.36	110.47
33	c1	516	BCR	C20-C19-C18	6.83	145.60	126.42
33	c1	517	BCR	C20-C19-C18	6.83	145.59	126.42
56	r1	626	ERG	C14-C13-C17	6.82	106.99	99.72
31	R1	602	CLA	O2D-CGD-CBD	6.81	123.38	111.27
42	c1	527	LMK	O2-C4-O3	-6.79	108.67	124.09
38	C1	524	DGA	CDB-CCB-CBB	-6.79	79.96	114.42
33	c	517	BCR	C20-C19-C18	6.78	145.47	126.42
38	b1	625	DGA	CDB-CCB-CBB	-6.71	80.36	114.42
38	b	623	DGA	CDB-CCB-CBB	-6.70	80.43	114.42
48	r	620	LUT	C21-C26-C27	6.68	121.15	112.70
38	c	524	DGA	CDB-CCB-CBB	-6.68	80.54	114.42
38	C	524	DGA	CDB-CCB-CBB	-6.67	80.58	114.42
50	R	622	NEX	C2-C1-C6	6.65	115.68	109.21
31	s1	603	CLA	O2D-CGD-CBD	6.60	123.00	111.27
31	S1	603	CLA	O2D-CGD-CBD	6.60	123.00	111.27
38	c1	524	DGA	CDB-CCB-CBB	-6.54	81.21	114.42
31	s	610	CLA	O2A-C1-C2	6.52	125.78	108.64
38	B1	625	DGA	CDB-CCB-CBB	-6.50	81.41	114.42
31	B1	606	CLA	CMD-C2D-C1D	6.48	136.14	124.71
31	b	609	CLA	O2D-CGD-CBD	6.47	122.76	111.27
33	B	619	BCR	C20-C19-C18	6.42	144.46	126.42
56	r1	626	ERG	C12-C13-C14	6.42	117.45	107.27
31	B1	609	CLA	O2D-CGD-CBD	6.42	122.67	111.27
42	c	627	LMK	O2-C4-O3	-6.41	109.54	124.09
49	r	622	XAT	C15-C14-C13	-6.41	118.16	127.31
31	b	607	CLA	CMD-C2D-C1D	6.38	135.96	124.71
48	n	621	LUT	C21-C26-C27	6.38	120.76	112.70
31	c	504	CLA	O2A-C1-C2	6.37	125.37	108.64
31	r	608	CLA	CMD-C2D-C1D	6.33	135.88	124.71
31	C	501	CLA	CMD-C2D-C1D	6.33	135.87	124.71
31	b	607	CLA	O2D-CGD-CBD	6.33	122.51	111.27
31	S	613	CLA	O2D-CGD-CBD	6.31	122.49	111.27
31	R1	604	CLA	O2A-C1-C2	6.31	123.73	108.97
31	C	506	CLA	O2D-CGD-CBD	6.30	122.47	111.27
31	Y1	613	CLA	CMD-C2D-C1D	6.29	135.80	124.71
42	C	527	LMK	O2-C4-O3	-6.29	109.81	124.09
37	b	620	C7Z	C11-C10-C9	-6.28	118.35	127.31
48	R1	620	LUT	C21-C26-C27	6.28	120.64	112.70
31	N	611	CLA	O2D-CGD-CBD	6.25	122.37	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	N1	622	XAT	C31-C30-C29	-6.24	118.40	127.31
31	y1	614	CLA	CMD-C2D-C1D	6.23	135.70	124.71
31	B	605	CLA	O2A-C1-C2	6.23	125.00	108.64
31	Y	604	CLA	O2D-CGD-CBD	6.22	122.33	111.27
37	B	620	C7Z	C11-C10-C9	-6.14	118.55	127.31
31	Y1	608	CLA	CMD-C2D-C1D	6.12	135.51	124.71
33	A1	411	BCR	C20-C19-C18	6.11	143.59	126.42
31	y	608	CLA	CMD-C2D-C1D	6.11	135.48	124.71
37	b1	620	C7Z	C15-C14-C13	-6.10	118.60	127.31
31	y	602	CLA	O2D-CGD-CBD	6.09	122.09	111.27
31	g1	614	CLA	O2A-C1-C2	6.09	123.20	108.97
31	C1	503	CLA	CMD-C2D-C1D	6.09	135.44	124.71
31	y1	608	CLA	CMD-C2D-C1D	6.08	135.42	124.71
31	B	617	CLA	O2A-C1-C2	6.04	124.50	108.64
31	b1	603	CLA	O2A-C1-C2	6.03	124.49	108.64
31	b1	608	CLA	O2A-C1-C2	6.02	124.45	108.64
48	g	621	LUT	C21-C26-C27	6.02	120.31	112.70
49	Y	622	XAT	C15-C14-C13	-6.00	118.74	127.31
31	s	605	CLA	O2D-CGD-CBD	6.00	121.94	111.27
31	C1	504	CLA	O2A-C1-C2	6.00	124.41	108.64
31	S1	614	CLA	CMD-C2D-C1D	5.99	135.28	124.71
48	s1	621	LUT	C21-C26-C27	5.99	120.28	112.70
31	R	604	CLA	O2A-C1-C2	5.97	122.93	108.97
31	C1	507	CLA	O2A-C1-C2	5.96	124.31	108.64
31	A1	405	CLA	CMD-C2D-C1D	5.96	135.22	124.71
31	g	604	CLA	CMD-C2D-C1D	5.95	135.19	124.71
31	r1	604	CLA	O2A-C1-C2	5.94	122.86	108.97
48	G1	621	LUT	C21-C26-C25	5.94	122.05	111.42
31	n	603	CLA	O2A-C1-C2	5.93	124.21	108.64
31	B1	608	CLA	CMD-C2D-C1D	5.92	135.15	124.71
31	R	612	CLA	CMD-C2D-C1D	5.92	135.14	124.71
31	s	614	CLA	O2A-C1-C2	5.92	124.18	108.64
31	N1	604	CLA	CMD-C2D-C1D	5.91	135.12	124.71
31	B	609	CLA	O2D-CGD-CBD	5.90	121.75	111.27
31	r1	609	CLA	O2A-C1-C2	5.89	124.12	108.64
31	N1	610	CLA	CMD-C2D-C1D	5.89	135.10	124.71
48	s	620	LUT	C21-C26-C27	5.89	120.15	112.70
31	y	604	CLA	O2A-C1-C2	5.88	124.09	108.64
31	c	510	CLA	CMD-C2D-C1D	5.88	135.07	124.71
31	c1	505	CLA	O2D-CGD-CBD	5.88	121.71	111.27
31	g1	610	CLA	CMD-C2D-C1D	5.88	135.07	124.71
31	N	604	CLA	O2D-CGD-CBD	5.87	121.70	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	511	CLA	CMD-C2D-C1D	5.87	135.06	124.71
31	B	606	CLA	CMD-C2D-C1D	5.86	135.05	124.71
49	R	621	XAT	C15-C14-C13	-5.86	118.94	127.31
31	N1	614	CLA	O2A-C1-C2	5.86	122.68	108.97
48	R	620	LUT	C21-C26-C27	5.86	120.10	112.70
56	R1	626	ERG	C14-C13-C17	5.85	105.97	99.72
31	Y1	602	CLA	CMD-C2D-C1D	5.85	135.02	124.71
48	N	621	LUT	C21-C26-C25	5.85	121.89	111.42
31	G	610	CLA	CMD-C2D-C1D	5.84	135.01	124.71
31	s	611	CLA	O2D-CGD-CBD	5.84	121.65	111.27
31	s	604	CLA	CMD-C2D-C1D	5.84	135.01	124.71
31	c	503	CLA	CMD-C2D-C1D	5.84	135.00	124.71
31	S1	602	CLA	O2D-CGD-CBD	5.83	121.63	111.27
33	d	404	BCR	C20-C19-C18	5.83	142.80	126.42
31	a	406	CLA	CMD-C2D-C1D	5.83	134.99	124.71
31	D1	402	CLA	O2A-C1-C2	5.83	123.95	108.64
31	s	610	CLA	CMD-C2D-C1D	5.82	134.98	124.71
50	r1	622	NEX	C2-C1-C6	5.82	114.87	109.21
31	y1	604	CLA	O2D-CGD-CBD	5.81	121.60	111.27
31	G1	611	CLA	CMD-C2D-C1D	5.81	134.96	124.71
31	A1	407	CLA	CMD-C2D-C1D	5.81	134.95	124.71
31	c	501	CLA	O2D-CGD-CBD	5.81	121.59	111.27
31	R1	608	CLA	CMD-C2D-C1D	5.81	134.95	124.71
31	C1	509	CLA	CMD-C2D-C1D	5.80	134.93	124.71
31	b	605	CLA	O2D-CGD-CBD	5.79	121.56	111.27
31	r	613	CLA	O2D-CGD-CBD	5.79	121.56	111.27
31	b	613	CLA	O2D-CGD-CBD	5.79	121.56	111.27
31	y	613	CLA	CMD-C2D-C1D	5.78	134.91	124.71
31	C	503	CLA	CMD-C2D-C1D	5.78	134.90	124.71
31	b	602	CLA	CMD-C2D-C1D	5.77	134.89	124.71
31	N1	603	CLA	CMD-C2D-C1D	5.77	134.89	124.71
31	c	509	CLA	CMD-C2D-C1D	5.77	134.88	124.71
31	C	501	CLA	O2D-CGD-CBD	5.77	121.52	111.27
31	S1	609	CLA	CMD-C2D-C1D	5.77	134.87	124.71
31	B1	616	CLA	CMD-C2D-C1D	5.76	134.87	124.71
31	B	605	CLA	CMD-C2D-C1D	5.76	134.87	124.71
31	C1	501	CLA	CMD-C2D-C1D	5.76	134.87	124.71
31	c1	511	CLA	O2A-C1-C2	5.75	123.75	108.64
46	h1	101	RRX	C1-C6-C5	-5.75	114.52	122.61
31	b1	613	CLA	CMD-C2D-C1D	5.75	134.84	124.71
31	y1	613	CLA	CMD-C2D-C1D	5.75	134.84	124.71
31	Y	602	CLA	O2D-CGD-CBD	5.74	121.47	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	613	CLA	O2D-CGD-CBD	5.74	121.47	111.27
31	c	502	CLA	O2A-C1-C2	5.74	123.73	108.64
31	S	605	CLA	O2A-C1-C2	5.74	123.71	108.64
31	N	610	CLA	O2D-CGD-CBD	5.74	121.46	111.27
31	C1	504	CLA	CMD-C2D-C1D	5.74	134.82	124.71
31	a1	405	CLA	CMD-C2D-C1D	5.73	134.81	124.71
31	C1	512	CLA	CMD-C2D-C1D	5.73	134.81	124.71
31	G	602	CLA	CMD-C2D-C1D	5.73	134.81	124.71
48	r1	620	LUT	C21-C26-C27	5.72	119.94	112.70
31	y1	610	CLA	CMD-C2D-C1D	5.72	134.80	124.71
31	b1	603	CLA	O2D-CGD-CBD	5.72	121.44	111.27
31	C	504	CLA	O2A-C1-C2	5.72	123.66	108.64
31	B1	612	CLA	O2A-C1-C2	5.72	123.66	108.64
31	r1	608	CLA	CMD-C2D-C1D	5.71	134.78	124.71
31	c	513	CLA	O2A-C1-C2	5.71	123.65	108.64
31	n	602	CLA	O2A-C1-C2	5.71	123.64	108.64
31	A1	406	CLA	CMD-C2D-C1D	5.70	134.77	124.71
31	B	609	CLA	CMD-C2D-C1D	5.70	134.76	124.71
31	d	402	CLA	O2A-C1-C2	5.70	123.62	108.64
31	B	615	CLA	O2A-C1-C2	5.70	123.62	108.64
31	C1	505	CLA	CMD-C2D-C1D	5.70	134.76	124.71
37	B1	620	C7Z	C38-C25-C26	-5.70	118.13	124.53
31	b	608	CLA	O2A-C1-C2	5.70	123.61	108.64
31	y	603	CLA	O2D-CGD-CBD	5.70	121.39	111.27
31	c1	504	CLA	O2A-C1-C2	5.69	123.59	108.64
48	R1	620	LUT	C35-C34-C33	-5.69	119.19	127.31
31	c	507	CLA	CMD-C2D-C1D	5.68	134.73	124.71
31	C	502	CLA	O2D-CGD-CBD	5.68	121.36	111.27
31	r	603	CLA	CMD-C2D-C1D	5.68	134.72	124.71
31	B1	607	CLA	CMD-C2D-C1D	5.68	134.72	124.71
31	c1	511	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	c1	503	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	G	613	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	n1	614	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	B	613	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	s	612	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	s	614	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	B	615	CLA	CMD-C2D-C1D	5.66	134.69	124.71
31	C	513	CLA	O2D-CGD-CBD	5.66	121.32	111.27
31	n	602	CLA	CMD-C2D-C1D	5.66	134.68	124.71
31	n1	602	CLA	CMD-C2D-C1D	5.65	134.68	124.71
31	G1	614	CLA	O2A-C1-C2	5.65	122.19	108.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	614	CLA	CMD-C2D-C1D	5.65	134.67	124.71
31	r	604	CLA	O2A-C1-C2	5.65	122.19	108.97
31	s1	612	CLA	CMD-C2D-C1D	5.65	134.67	124.71
31	C	506	CLA	CMD-C2D-C1D	5.65	134.67	124.71
31	B1	614	CLA	CMD-C2D-C1D	5.65	134.67	124.71
31	R	608	CLA	CMD-C2D-C1D	5.65	134.66	124.71
33	D	404	BCR	C20-C19-C18	5.65	142.28	126.42
31	N1	604	CLA	O2A-C1-C2	5.65	123.47	108.64
31	n	604	CLA	O2A-C1-C2	5.64	123.47	108.64
49	g	622	XAT	C15-C14-C13	-5.64	119.26	127.31
31	G1	603	CLA	CMD-C2D-C1D	5.64	134.66	124.71
43	D1	401	BCT	O2-C-O1	5.64	134.18	119.55
31	n	603	CLA	CMD-C2D-C1D	5.64	134.65	124.71
31	c1	510	CLA	CMD-C2D-C1D	5.64	134.65	124.71
31	N	604	CLA	CMD-C2D-C1D	5.64	134.65	124.71
46	h	101	RRX	C15-C14-C13	-5.64	119.26	127.31
31	A	410	CLA	CMD-C2D-C1D	5.64	134.65	124.71
48	R	620	LUT	C31-C30-C29	-5.64	119.27	127.31
31	c1	513	CLA	O2A-C1-C2	5.64	123.45	108.64
49	N1	622	XAT	C15-C14-C13	-5.63	119.27	127.31
31	a1	407	CLA	O2D-CGD-CBD	5.63	121.27	111.27
31	r	611	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	Y	608	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	s	617	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	B	607	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	B1	606	CLA	O2A-C1-C2	5.63	123.42	108.64
31	b1	604	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	g1	611	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	b	615	CLA	CMD-C2D-C1D	5.62	134.62	124.71
31	G1	610	CLA	CMD-C2D-C1D	5.62	134.62	124.71
31	c1	501	CLA	O2A-C1-C2	5.62	123.41	108.64
31	n	612	CLA	CMD-C2D-C1D	5.62	134.62	124.71
31	y	608	CLA	O2A-C1-C2	5.62	123.40	108.64
31	G	604	CLA	CMD-C2D-C1D	5.61	134.61	124.71
31	b	608	CLA	CMD-C2D-C1D	5.61	134.61	124.71
31	R	603	CLA	O2D-CGD-CBD	5.61	121.24	111.27
31	B	614	CLA	CMD-C2D-C1D	5.61	134.60	124.71
31	Y	603	CLA	O2D-CGD-CBD	5.61	121.24	111.27
31	g	610	CLA	CMD-C2D-C1D	5.61	134.60	124.71
31	n1	603	CLA	O2D-CGD-CBD	5.61	121.23	111.27
31	r1	603	CLA	O2A-C1-C2	5.61	123.37	108.64
31	r1	610	CLA	O2A-C1-C2	5.60	123.36	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	612	CLA	O2D-CGD-CBD	5.60	121.22	111.27
31	c	501	CLA	CMD-C2D-C1D	5.60	134.59	124.71
31	S1	604	CLA	O2A-C1-C2	5.60	123.36	108.64
31	d	403	CLA	O2D-CGD-CBD	5.60	121.22	111.27
31	N	613	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	R1	604	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	r1	612	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	n1	614	CLA	O2A-C1-C2	5.60	122.06	108.97
31	C1	507	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	A	406	CLA	CMD-C2D-C1D	5.60	134.58	124.71
46	H	101	RRX	C11-C10-C9	-5.59	119.33	127.31
31	R1	612	CLA	CMD-C2D-C1D	5.59	134.56	124.71
31	R	611	CLA	CMD-C2D-C1D	5.59	134.56	124.71
31	B1	610	CLA	O2A-C1-C2	5.58	123.31	108.64
31	Y	614	CLA	CMD-C2D-C1D	5.58	134.55	124.71
49	n	622	XAT	C15-C14-C13	-5.58	119.34	127.31
31	c	506	CLA	CMD-C2D-C1D	5.58	134.55	124.71
49	n	622	XAT	C31-C30-C29	-5.58	119.35	127.31
31	a1	407	CLA	CMD-C2D-C1D	5.58	134.54	124.71
31	S	605	CLA	O2D-CGD-CBD	5.58	121.18	111.27
31	c	513	CLA	O2D-CGD-CBD	5.58	121.18	111.27
31	r1	604	CLA	CMD-C2D-C1D	5.58	134.54	124.71
31	g	612	CLA	O2D-CGD-CBD	5.58	121.17	111.27
31	B	608	CLA	CMD-C2D-C1D	5.57	134.54	124.71
43	D	401	BCT	O2-C-O1	5.57	134.00	119.55
31	b1	605	CLA	CMD-C2D-C1D	5.57	134.53	124.71
31	C1	508	CLA	O2A-C1-C2	5.57	123.27	108.64
31	B	603	CLA	CMD-C2D-C1D	5.57	134.53	124.71
31	C	509	CLA	CMD-C2D-C1D	5.57	134.52	124.71
31	S	605	CLA	CMD-C2D-C1D	5.57	134.52	124.71
31	c1	509	CLA	CMD-C2D-C1D	5.57	134.52	124.71
31	R	610	CLA	CMD-C2D-C1D	5.56	134.52	124.71
31	n	610	CLA	O2A-C1-C2	5.56	123.25	108.64
31	a1	406	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	a	407	CLA	O2A-C1-C2	5.56	121.97	108.97
31	S1	603	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	s1	602	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	d1	403	CLA	CMD-C2D-C1D	5.56	134.51	124.71
48	N1	621	LUT	C21-C26-C27	5.56	119.72	112.70
31	G	604	CLA	O2D-CGD-CBD	5.55	121.14	111.27
31	b1	608	CLA	CMD-C2D-C1D	5.55	134.50	124.71
48	N1	621	LUT	C21-C26-C25	5.55	121.36	111.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	612	CLA	CMD-C2D-C1D	5.55	134.50	124.71
31	n	602	CLA	O2D-CGD-CBD	5.55	121.13	111.27
31	R	609	CLA	CMD-C2D-C1D	5.55	134.49	124.71
31	c1	507	CLA	O2A-C1-C2	5.55	123.22	108.64
31	y	610	CLA	CMD-C2D-C1D	5.55	134.49	124.71
31	s1	605	CLA	O2A-C1-C2	5.55	123.21	108.64
31	G	611	CLA	O2D-CGD-CBD	5.55	121.12	111.27
31	g1	612	CLA	CMD-C2D-C1D	5.55	134.49	124.71
31	b1	614	CLA	CMD-C2D-C1D	5.55	134.49	124.71
31	n	613	CLA	O2A-C1-C2	5.54	123.20	108.64
31	r	604	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	Y	610	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	a1	405	CLA	O2A-C1-C2	5.54	123.20	108.64
31	b	614	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	b1	606	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	B1	605	CLA	O2A-C1-C2	5.54	123.19	108.64
48	y	620	LUT	C21-C26-C25	5.54	121.34	111.42
31	G	611	CLA	CMD-C2D-C1D	5.54	134.47	124.71
31	C	504	CLA	O2D-CGD-CBD	5.53	121.10	111.27
31	b	606	CLA	CMD-C2D-C1D	5.53	134.47	124.71
31	G1	603	CLA	O2A-C1-C2	5.53	123.18	108.64
31	G	603	CLA	CMD-C2D-C1D	5.53	134.47	124.71
31	B1	608	CLA	O2A-C1-C2	5.53	123.18	108.64
31	A	407	CLA	O2A-C1-C2	5.53	121.90	108.97
31	G1	613	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	G1	613	CLA	O2A-C1-C2	5.53	123.17	108.64
31	s1	604	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	C	510	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	b1	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	R	613	CLA	CMD-C2D-C1D	5.53	134.45	124.71
31	B1	602	CLA	CMD-C2D-C1D	5.53	134.45	124.71
31	S1	604	CLA	O2D-CGD-CBD	5.53	121.09	111.27
31	C	508	CLA	O2A-C1-C2	5.53	123.16	108.64
31	G	602	CLA	O2D-CGD-CBD	5.52	121.08	111.27
31	n1	604	CLA	CMD-C2D-C1D	5.52	134.45	124.71
31	n	614	CLA	O2A-C1-C2	5.52	121.88	108.97
31	B1	613	CLA	O2D-CGD-CBD	5.52	121.08	111.27
31	B	616	CLA	O2D-CGD-CBD	5.52	121.08	111.27
37	B1	620	C7Z	C15-C14-C13	-5.52	119.43	127.31
31	s1	605	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	A	405	CLA	CMD-C2D-C1D	5.52	134.43	124.71
31	C	502	CLA	O2A-C1-C2	5.51	123.12	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y1	612	CLA	O2D-CGD-CBD	5.51	121.06	111.27
31	c	506	CLA	O2D-CGD-CBD	5.51	121.06	111.27
31	g1	603	CLA	CMD-C2D-C1D	5.51	134.42	124.71
48	g1	621	LUT	C21-C26-C25	5.51	121.28	111.42
31	Y1	611	CLA	CMD-C2D-C1D	5.51	134.42	124.71
49	r	622	XAT	C7-C8-C9	-5.51	116.99	125.53
31	g	602	CLA	CMD-C2D-C1D	5.51	134.42	124.71
48	y1	621	LUT	C35-C34-C33	-5.51	119.45	127.31
31	b	610	CLA	O2A-C1-C2	5.50	123.10	108.64
56	R1	626	ERG	C12-C13-C14	5.50	116.00	107.27
31	c1	506	CLA	O2D-CGD-CBD	5.50	121.05	111.27
31	g	613	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	S	611	CLA	O2D-CGD-CBD	5.50	121.04	111.27
31	y	612	CLA	O2D-CGD-CBD	5.50	121.04	111.27
31	g	611	CLA	O2D-CGD-CBD	5.50	121.04	111.27
31	n1	610	CLA	CMD-C2D-C1D	5.50	134.40	124.71
31	b1	605	CLA	O2A-C1-C2	5.50	123.08	108.64
31	Y	604	CLA	CMD-C2D-C1D	5.50	134.40	124.71
31	s1	617	CLA	CMD-C2D-C1D	5.50	134.40	124.71
31	y1	603	CLA	O2D-CGD-CBD	5.49	121.03	111.27
31	Y1	614	CLA	O2D-CGD-CBD	5.49	121.03	111.27
48	S1	620	LUT	C35-C34-C33	-5.49	119.48	127.31
48	Y	620	LUT	C21-C26-C25	5.49	121.25	111.42
31	S1	605	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	n1	603	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	g	610	CLA	O2A-C1-C2	5.49	123.06	108.64
31	S	613	CLA	CMD-C2D-C1D	5.49	134.38	124.71
43	d	401	BCT	O2-C-O1	5.49	133.78	119.55
31	D	402	CLA	CMD-C2D-C1D	5.49	134.38	124.71
31	c	511	CLA	CMD-C2D-C1D	5.49	134.38	124.71
31	S1	605	CLA	O2A-C1-C2	5.49	123.05	108.64
31	C1	505	CLA	O2A-C1-C2	5.48	123.05	108.64
44	d1	405	PL9	C7-C3-C4	5.48	121.33	116.88
31	g1	613	CLA	CMD-C2D-C1D	5.48	134.38	124.71
31	s	611	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	N1	603	CLA	O2A-C1-C2	5.48	123.04	108.64
31	C1	511	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	C	507	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	N1	611	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	a	405	CLA	O2A-C1-C2	5.48	123.03	108.64
31	C1	510	CLA	CMD-C2D-C1D	5.48	134.36	124.71
31	G	604	CLA	O2A-C1-C2	5.48	121.78	108.97

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D1	403	CLA	CMD-C2D-C1D	5.47	134.36	124.71
31	c	512	CLA	O2A-C1-C2	5.47	123.02	108.64
31	y1	611	CLA	O2A-C1-C2	5.47	123.02	108.64
31	n1	602	CLA	O2A-C1-C2	5.47	123.02	108.64
31	g	614	CLA	O2A-C1-C2	5.47	121.77	108.97
31	N	604	CLA	O2A-C1-C2	5.47	123.02	108.64
48	S1	620	LUT	C21-C26-C27	5.47	119.62	112.70
31	Y	611	CLA	CMD-C2D-C1D	5.47	134.36	124.71
31	N1	604	CLA	O2D-CGD-CBD	5.47	120.99	111.27
31	c1	511	CLA	O2D-CGD-CBD	5.47	120.99	111.27
31	n	611	CLA	CMD-C2D-C1D	5.47	134.35	124.71
31	b	605	CLA	CMD-C2D-C1D	5.47	134.35	124.71
31	y	611	CLA	O2D-CGD-CBD	5.47	120.98	111.27
31	G	610	CLA	O2D-CGD-CBD	5.47	120.98	111.27
31	s1	611	CLA	CMD-C2D-C1D	5.47	134.34	124.71
31	A	407	CLA	CMD-C2D-C1D	5.46	134.34	124.71
48	y	621	LUT	C21-C26-C25	5.45	121.19	111.42
31	G1	610	CLA	O2A-C1-C2	5.45	122.96	108.64
31	c1	502	CLA	CMD-C2D-C1D	5.45	134.32	124.71
31	g	614	CLA	CMD-C2D-C1D	5.45	134.32	124.71
31	c	507	CLA	O2D-CGD-CBD	5.45	120.95	111.27
31	B1	604	CLA	CMD-C2D-C1D	5.45	134.31	124.71
48	n1	621	LUT	C7-C8-C9	-5.45	118.01	126.23
31	y1	603	CLA	CMD-C2D-C1D	5.44	134.31	124.71
31	G1	604	CLA	CMD-C2D-C1D	5.44	134.31	124.71
31	S1	604	CLA	CMD-C2D-C1D	5.44	134.31	124.71
31	B	602	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	Y	603	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	g	611	CLA	CMD-C2D-C1D	5.43	134.29	124.71
31	s1	613	CLA	CMD-C2D-C1D	5.43	134.29	124.71
31	g1	604	CLA	O2D-CGD-CBD	5.43	120.92	111.27
31	s1	603	CLA	CMD-C2D-C1D	5.43	134.29	124.71
31	s	609	CLA	CMD-C2D-C1D	5.43	134.29	124.71
31	s1	609	CLA	O2D-CGD-CBD	5.43	120.92	111.27
31	y	614	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	R	602	CLA	O2D-CGD-CBD	5.43	120.92	111.27
31	N	613	CLA	O2A-C1-C2	5.43	122.91	108.64
31	r	612	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	g1	603	CLA	O2A-C1-C2	5.43	122.90	108.64
31	D	403	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	b1	616	CLA	CMD-C2D-C1D	5.43	134.28	124.71
48	s1	621	LUT	C35-C34-C33	-5.42	119.57	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	611	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	c1	513	CLA	O2D-CGD-CBD	5.42	120.90	111.27
50	g1	623	NEX	C17-C1-C6	-5.42	105.62	110.47
31	R	604	CLA	CMD-C2D-C1D	5.42	134.27	124.71
48	G	620	LUT	C21-C26-C27	5.42	119.55	112.70
31	G	602	CLA	O2A-C1-C2	5.42	122.87	108.64
31	c1	507	CLA	CMD-C2D-C1D	5.41	134.26	124.71
31	C	504	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	a	410	CLA	O2D-CGD-CBD	5.41	120.89	111.27
48	Y1	620	LUT	C21-C26-C25	5.41	121.11	111.42
31	R	603	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	G1	612	CLA	O2D-CGD-CBD	5.41	120.88	111.27
50	R1	622	NEX	C17-C1-C6	-5.41	105.63	110.47
31	b	603	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	B1	605	CLA	CMD-C2D-C1D	5.41	134.24	124.71
31	Y1	603	CLA	O2D-CGD-CBD	5.41	120.88	111.27
48	s	620	LUT	C21-C26-C25	5.41	121.10	111.42
31	N1	612	CLA	CMD-C2D-C1D	5.41	134.24	124.71
46	H	101	RRX	C7-C8-C9	-5.40	118.07	126.23
48	G1	621	LUT	C7-C8-C9	-5.40	118.07	126.23
31	B	610	CLA	O2D-CGD-CBD	5.40	120.86	111.27
31	b	609	CLA	CMD-C2D-C1D	5.40	134.23	124.71
31	r	609	CLA	O2A-C1-C2	5.40	122.83	108.64
31	Y	612	CLA	O2D-CGD-CBD	5.40	120.86	111.27
31	B	611	CLA	O2A-C1-C2	5.40	122.82	108.64
33	D1	404	BCR	C20-C19-C18	5.40	141.58	126.42
31	N1	614	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	g1	602	CLA	O2A-C1-C2	5.39	122.81	108.64
31	r1	602	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	S	604	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	n	604	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	D	402	CLA	O2A-C1-C2	5.39	122.80	108.64
31	c	504	CLA	CMD-C2D-C1D	5.39	134.21	124.71
31	b1	615	CLA	CMD-C2D-C1D	5.39	134.21	124.71
31	R1	609	CLA	O2A-C1-C2	5.39	122.79	108.64
31	n	611	CLA	O2A-C1-C2	5.39	121.57	108.97
48	r	620	LUT	C31-C30-C29	-5.39	119.62	127.31
49	y	622	XAT	C31-C30-C29	-5.39	119.62	127.31
31	Y1	614	CLA	CMD-C2D-C1D	5.38	134.20	124.71
31	g	602	CLA	O2A-C1-C2	5.38	122.78	108.64
48	n1	621	LUT	C21-C26-C25	5.38	121.06	111.42
31	n1	612	CLA	CMD-C2D-C1D	5.38	134.19	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	614	CLA	O2A-C1-C2	5.38	121.55	108.97
31	s	602	CLA	CMD-C2D-C1D	5.38	134.19	124.71
31	b1	602	CLA	CMD-C2D-C1D	5.37	134.18	124.71
31	s	602	CLA	O2A-C1-C2	5.37	122.75	108.64
31	b	603	CLA	O2A-C1-C2	5.37	122.75	108.64
31	G	614	CLA	O2A-C1-C2	5.37	121.52	108.97
31	S1	603	CLA	O2A-C1-C2	5.37	122.74	108.64
31	B1	610	CLA	CMD-C2D-C1D	5.37	134.17	124.71
31	C	513	CLA	O2A-C1-C2	5.36	122.73	108.64
31	B1	615	CLA	CMD-C2D-C1D	5.36	134.17	124.71
48	Y1	621	LUT	C21-C26-C25	5.36	121.02	111.42
48	G	621	LUT	C21-C26-C27	5.36	119.48	112.70
31	r	613	CLA	CMD-C2D-C1D	5.36	134.16	124.71
31	y1	611	CLA	CMD-C2D-C1D	5.36	134.16	124.71
46	h1	101	RRX	C24-C23-C22	5.36	134.33	126.23
31	R1	603	CLA	CMD-C2D-C1D	5.36	134.16	124.71
31	b	611	CLA	CMD-C2D-C1D	5.36	134.16	124.71
31	c	510	CLA	O2D-CGD-CBD	5.36	120.79	111.27
50	S1	623	NEX	C17-C1-C6	-5.35	105.68	110.47
31	r1	612	CLA	O2A-C1-C2	5.35	122.70	108.64
31	c1	501	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	B	605	CLA	O2D-CGD-CBD	5.35	120.77	111.27
31	b1	612	CLA	O2A-C1-C2	5.35	122.69	108.64
48	y1	620	LUT	C21-C26-C25	5.34	120.99	111.42
49	Y	622	XAT	C31-C30-C29	-5.34	119.69	127.31
31	n	613	CLA	CMD-C2D-C1D	5.34	134.12	124.71
31	y1	602	CLA	O2D-CGD-CBD	5.34	120.75	111.27
31	n1	611	CLA	O2A-C1-C2	5.34	121.45	108.97
31	n	610	CLA	CMD-C2D-C1D	5.34	134.12	124.71
31	S	609	CLA	CMD-C2D-C1D	5.34	134.12	124.71
31	g1	604	CLA	CMD-C2D-C1D	5.33	134.11	124.71
31	c	501	CLA	O2A-C1-C2	5.33	122.65	108.64
31	b1	607	CLA	O2D-CGD-CBD	5.33	120.74	111.27
31	r	602	CLA	CMD-C2D-C1D	5.33	134.11	124.71
31	b1	617	CLA	CMD-C2D-C1D	5.33	134.11	124.71
31	Y1	604	CLA	CMD-C2D-C1D	5.33	134.11	124.71
31	c1	504	CLA	CMD-C2D-C1D	5.33	134.11	124.71
31	s1	602	CLA	O2D-CGD-CBD	5.33	120.74	111.27
31	N	602	CLA	CMD-C2D-C1D	5.33	134.10	124.71
31	y	611	CLA	CMD-C2D-C1D	5.33	134.10	124.71
31	B	606	CLA	O2A-C1-C2	5.33	122.64	108.64
31	g	602	CLA	O2D-CGD-CBD	5.33	120.73	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	613	CLA	O2A-C1-C2	5.32	122.63	108.64
49	R1	621	XAT	C31-C30-C29	-5.32	119.71	127.31
48	s1	620	LUT	C21-C26-C25	5.32	120.94	111.42
31	S1	602	CLA	O2A-C1-C2	5.32	122.61	108.64
31	B	604	CLA	CMD-C2D-C1D	5.31	134.08	124.71
31	y1	602	CLA	CMD-C2D-C1D	5.31	134.08	124.71
31	B	607	CLA	O2D-CGD-CBD	5.31	120.71	111.27
31	S1	612	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	r1	602	CLA	O2D-CGD-CBD	5.31	120.71	111.27
31	n	604	CLA	O2D-CGD-CBD	5.31	120.71	111.27
31	y	614	CLA	O2D-CGD-CBD	5.31	120.70	111.27
31	S	614	CLA	O2D-CGD-CBD	5.31	120.70	111.27
31	c1	512	CLA	O2A-C1-C2	5.31	122.59	108.64
37	B	620	C7Z	C15-C14-C13	-5.31	119.73	127.31
31	s	605	CLA	O2A-C1-C2	5.31	122.58	108.64
48	n	620	LUT	C7-C8-C9	-5.31	118.22	126.23
31	c	512	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	y	610	CLA	O2A-C1-C2	5.31	122.58	108.64
31	b	615	CLA	O2A-C1-C2	5.31	122.58	108.64
31	A	410	CLA	O2D-CGD-CBD	5.31	120.70	111.27
31	S1	609	CLA	O2D-CGD-CBD	5.31	120.70	111.27
49	n1	622	XAT	C15-C14-C13	-5.31	119.74	127.31
31	N1	613	CLA	O2A-C1-C2	5.31	122.58	108.64
31	y	610	CLA	O2D-CGD-CBD	5.31	120.69	111.27
31	C1	506	CLA	CMD-C2D-C1D	5.30	134.06	124.71
46	H	101	RRX	C16-C17-C18	-5.30	119.74	127.31
31	c1	513	CLA	CMD-C2D-C1D	5.30	134.06	124.71
31	a1	407	CLA	O2A-C1-C2	5.30	121.36	108.97
31	C1	513	CLA	CMD-C2D-C1D	5.30	134.05	124.71
31	n	611	CLA	O2D-CGD-CBD	5.30	120.68	111.27
31	c	510	CLA	O2A-C1-C2	5.30	122.56	108.64
49	r1	621	XAT	C38-C25-C24	5.30	120.24	114.28
31	n1	611	CLA	CMD-C2D-C1D	5.30	134.04	124.71
31	G	610	CLA	O2A-C1-C2	5.29	122.55	108.64
31	r1	608	CLA	O2A-C1-C2	5.29	122.54	108.64
31	R	604	CLA	O2D-CGD-CBD	5.29	120.67	111.27
31	S	613	CLA	O2A-C1-C2	5.29	122.54	108.64
31	g1	611	CLA	O2A-C1-C2	5.29	122.54	108.64
31	c1	512	CLA	O2D-CGD-CBD	5.29	120.66	111.27
31	b	616	CLA	CMD-C2D-C1D	5.29	134.03	124.71
31	B	616	CLA	CMD-C2D-C1D	5.29	134.03	124.71
31	r	610	CLA	CMD-C2D-C1D	5.28	134.02	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	606	CLA	O2D-CGD-CBD	5.28	120.65	111.27
31	B1	604	CLA	O2A-C1-C2	5.28	122.52	108.64
31	D	403	CLA	O2D-CGD-CBD	5.28	120.65	111.27
31	c1	503	CLA	O2D-CGD-CBD	5.28	120.65	111.27
31	y1	612	CLA	CMD-C2D-C1D	5.28	134.02	124.71
31	S	609	CLA	O2D-CGD-CBD	5.28	120.64	111.27
31	c	502	CLA	CMD-C2D-C1D	5.28	134.01	124.71
31	Y	610	CLA	O2D-CGD-CBD	5.27	120.64	111.27
48	y	620	LUT	C35-C34-C33	-5.27	119.79	127.31
31	b	604	CLA	CMD-C2D-C1D	5.27	134.00	124.71
31	C1	501	CLA	O2A-C1-C2	5.27	122.49	108.64
31	R	602	CLA	O2A-C1-C2	5.27	122.49	108.64
31	n1	604	CLA	O2A-C1-C2	5.27	122.48	108.64
48	N1	620	LUT	C21-C26-C25	5.27	120.86	111.42
31	A	410	CLA	O2A-C1-C2	5.27	122.48	108.64
31	Y1	612	CLA	O2D-CGD-CBD	5.27	120.63	111.27
31	N	614	CLA	CMD-C2D-C1D	5.27	134.00	124.71
31	a	407	CLA	CMD-C2D-C1D	5.27	133.99	124.71
31	B1	617	CLA	CMD-C2D-C1D	5.27	133.99	124.71
31	B1	603	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	b	617	CLA	O2A-C1-C2	5.26	122.47	108.64
31	y1	604	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	C	502	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	B1	611	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	Y1	603	CLA	O2A-C1-C2	5.26	122.46	108.64
31	b	612	CLA	O2D-CGD-CBD	5.26	120.61	111.27
31	Y1	610	CLA	O2A-C1-C2	5.26	122.45	108.64
31	g1	614	CLA	CMD-C2D-C1D	5.26	133.97	124.71
31	N1	611	CLA	O2A-C1-C2	5.25	121.26	108.97
31	A1	410	CLA	CMD-C2D-C1D	5.25	133.97	124.71
31	G	612	CLA	CMD-C2D-C1D	5.25	133.97	124.71
31	R1	602	CLA	CMD-C2D-C1D	5.25	133.97	124.71
31	b1	610	CLA	CMD-C2D-C1D	5.25	133.97	124.71
31	n	614	CLA	O2D-CGD-CBD	5.25	120.60	111.27
31	G1	604	CLA	O2A-C1-C2	5.24	121.23	108.97
48	S1	621	LUT	C7-C8-C9	-5.24	118.31	126.23
46	H1	101	RRX	C37-C22-C23	5.24	126.34	118.08
31	C	510	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	a1	410	CLA	CMD-C2D-C1D	5.24	133.95	124.71
31	N	603	CLA	O2D-CGD-CBD	5.24	120.58	111.27
48	G	621	LUT	C31-C30-C29	-5.24	119.83	127.31
31	s	605	CLA	CMD-C2D-C1D	5.24	133.95	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g1	612	CLA	O2D-CGD-CBD	5.24	120.58	111.27
46	H	101	RRX	C15-C14-C13	-5.24	119.83	127.31
44	D	405	PL9	C7-C3-C4	5.24	121.13	116.88
31	y	602	CLA	O2A-C1-C2	5.24	122.39	108.64
31	D1	403	CLA	O2D-CGD-CBD	5.23	120.57	111.27
40	B1	623	DGD	O2G-C1B-C2B	5.23	122.78	111.50
50	s	623	NEX	C2-C1-C6	5.23	114.30	109.21
31	B	609	CLA	O2A-C1-C2	5.23	122.39	108.64
31	s1	610	CLA	CMD-C2D-C1D	5.23	133.93	124.71
31	C1	502	CLA	CMD-C2D-C1D	5.23	133.93	124.71
31	S	617	CLA	O2A-C1-C2	5.23	122.38	108.64
31	y1	610	CLA	O2A-C1-C2	5.23	122.38	108.64
31	S1	613	CLA	CMD-C2D-C1D	5.23	133.93	124.71
48	y1	621	LUT	C21-C26-C27	5.22	119.30	112.70
31	R	610	CLA	O2D-CGD-CBD	5.22	120.55	111.27
31	b	613	CLA	CMD-C2D-C1D	5.22	133.91	124.71
31	S1	613	CLA	O2A-C1-C2	5.22	122.35	108.64
43	d1	401	BCT	O2-C-O1	5.22	133.08	119.55
31	s1	611	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	D1	402	CLA	CMD-C2D-C1D	5.21	133.90	124.71
31	N	603	CLA	CMD-C2D-C1D	5.21	133.90	124.71
31	R	602	CLA	CMD-C2D-C1D	5.21	133.90	124.71
31	S	612	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	C1	512	CLA	O2A-C1-C2	5.21	122.33	108.64
31	b1	616	CLA	O2A-C1-C2	5.21	122.33	108.64
31	S	602	CLA	CMD-C2D-C1D	5.21	133.89	124.71
31	y	604	CLA	CMD-C2D-C1D	5.21	133.89	124.71
31	Y	614	CLA	O2A-C1-C2	5.21	122.32	108.64
31	n1	602	CLA	O2D-CGD-CBD	5.21	120.52	111.27
31	Y	610	CLA	O2A-C1-C2	5.21	122.32	108.64
31	s1	609	CLA	O2A-C1-C2	5.21	122.31	108.64
48	G1	620	LUT	C21-C26-C25	5.21	120.74	111.42
31	s	603	CLA	CMD-C2D-C1D	5.20	133.88	124.71
31	r	602	CLA	O2D-CGD-CBD	5.20	120.51	111.27
31	r	612	CLA	O2D-CGD-CBD	5.20	120.51	111.27
31	n	614	CLA	CMD-C2D-C1D	5.20	133.88	124.71
31	c1	501	CLA	O2D-CGD-CBD	5.20	120.51	111.27
31	R1	612	CLA	O2A-C1-C2	5.20	122.30	108.64
31	Y1	604	CLA	O2D-CGD-CBD	5.20	120.51	111.27
31	r	612	CLA	O2A-C1-C2	5.20	122.30	108.64
31	S	610	CLA	CMD-C2D-C1D	5.20	133.87	124.71
48	N	620	LUT	C21-C26-C25	5.20	120.73	111.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y1	612	CLA	CMD-C2D-C1D	5.20	133.87	124.71
48	n1	621	LUT	C11-C10-C9	-5.20	119.89	127.31
31	b1	609	CLA	CMD-C2D-C1D	5.20	133.87	124.71
31	a	405	CLA	CMD-C2D-C1D	5.19	133.86	124.71
31	B1	603	CLA	O2D-CGD-CBD	5.19	120.49	111.27
31	C	513	CLA	CMD-C2D-C1D	5.19	133.86	124.71
31	B	604	CLA	O2A-C1-C2	5.19	122.27	108.64
31	C1	503	CLA	O2D-CGD-CBD	5.19	120.49	111.27
31	r	609	CLA	CMD-C2D-C1D	5.19	133.86	124.71
31	G1	602	CLA	O2A-C1-C2	5.19	122.27	108.64
31	a	410	CLA	CMD-C2D-C1D	5.19	133.85	124.71
31	B	615	CLA	O2D-CGD-CBD	5.19	120.48	111.27
31	d1	403	CLA	O2A-C1-C2	5.19	122.26	108.64
31	c1	506	CLA	CMD-C2D-C1D	5.18	133.85	124.71
31	b	611	CLA	O2A-C1-C2	5.18	122.26	108.64
31	B	603	CLA	O2D-CGD-CBD	5.18	120.47	111.27
31	n1	613	CLA	CMD-C2D-C1D	5.18	133.84	124.71
31	G	603	CLA	O2D-CGD-CBD	5.18	120.47	111.27
31	B	603	CLA	O2A-C1-C2	5.18	122.24	108.64
31	c	505	CLA	O2A-C1-C2	5.18	122.24	108.64
48	n1	621	LUT	C21-C26-C27	5.18	119.24	112.70
31	b1	613	CLA	O2D-CGD-CBD	5.17	120.46	111.27
31	s	613	CLA	O2A-C1-C2	5.17	122.23	108.64
31	y	603	CLA	CMD-C2D-C1D	5.17	133.83	124.71
31	a1	410	CLA	O2D-CGD-CBD	5.17	120.46	111.27
31	b1	607	CLA	O2A-C1-C2	5.17	122.23	108.64
31	R	611	CLA	O2D-CGD-CBD	5.17	120.46	111.27
31	g	604	CLA	O2A-C1-C2	5.17	121.06	108.97
31	S1	614	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	d	402	CLA	CMD-C2D-C1D	5.17	133.82	124.71
31	R	610	CLA	O2A-C1-C2	5.17	122.22	108.64
31	S	603	CLA	CMD-C2D-C1D	5.17	133.82	124.71
31	s1	604	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	r	604	CLA	O2D-CGD-CBD	5.17	120.45	111.27
48	y1	621	LUT	C21-C26-C25	5.17	120.67	111.42
49	n1	622	XAT	C31-C30-C29	-5.17	119.94	127.31
31	b1	605	CLA	O2D-CGD-CBD	5.16	120.45	111.27
31	N1	610	CLA	O2D-CGD-CBD	5.16	120.44	111.27
31	G	614	CLA	O2D-CGD-CBD	5.16	120.44	111.27
31	g	614	CLA	O2D-CGD-CBD	5.16	120.44	111.27
31	g	603	CLA	CMD-C2D-C1D	5.16	133.81	124.71
31	D	403	CLA	O2A-C1-C2	5.16	122.20	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	610	CLA	O2D-CGD-CBD	5.16	120.44	111.27
31	N1	613	CLA	CMD-C2D-C1D	5.16	133.80	124.71
31	Y	602	CLA	O2A-C1-C2	5.16	122.18	108.64
31	b	602	CLA	O2A-C1-C2	5.15	122.18	108.64
31	b1	607	CLA	CMD-C2D-C1D	5.15	133.78	124.71
48	S	620	LUT	C21-C26-C27	5.15	119.20	112.70
31	C	508	CLA	CMD-C2D-C1D	5.14	133.78	124.71
31	y1	612	CLA	O2A-C1-C2	5.14	122.16	108.64
31	Y	614	CLA	O2D-CGD-CBD	5.14	120.41	111.27
31	G1	614	CLA	CMD-C2D-C1D	5.14	133.78	124.71
31	G1	611	CLA	O2D-CGD-CBD	5.14	120.41	111.27
31	b	610	CLA	CMD-C2D-C1D	5.14	133.77	124.71
31	b	611	CLA	O2D-CGD-CBD	5.14	120.40	111.27
31	s1	605	CLA	O2D-CGD-CBD	5.14	120.40	111.27
31	b	612	CLA	O2A-C1-C2	5.14	122.13	108.64
48	g	620	LUT	C21-C26-C25	5.13	120.61	111.42
48	Y	621	LUT	C21-C26-C25	5.13	120.61	111.42
49	Y1	622	XAT	C15-C14-C13	-5.13	119.99	127.31
31	c	506	CLA	O2A-C1-C2	5.13	122.12	108.64
31	g1	602	CLA	O2D-CGD-CBD	5.13	120.39	111.27
31	s1	610	CLA	O2D-CGD-CBD	5.13	120.39	111.27
31	g1	613	CLA	O2A-C1-C2	5.13	122.12	108.64
31	g1	602	CLA	CMD-C2D-C1D	5.13	133.75	124.71
31	n1	613	CLA	O2A-C1-C2	5.13	122.11	108.64
31	G	613	CLA	O2D-CGD-CBD	5.13	120.38	111.27
31	Y1	602	CLA	O2A-C1-C2	5.12	122.10	108.64
31	a	407	CLA	O2D-CGD-CBD	5.12	120.37	111.27
31	Y1	603	CLA	CMD-C2D-C1D	5.12	133.74	124.71
31	n1	603	CLA	O2A-C1-C2	5.12	122.09	108.64
31	b1	611	CLA	O2D-CGD-CBD	5.12	120.37	111.27
31	S1	617	CLA	O2A-C1-C2	5.12	122.09	108.64
33	c1	514	BCR	C15-C14-C13	-5.12	120.00	127.31
31	n1	604	CLA	O2D-CGD-CBD	5.12	120.36	111.27
48	g	621	LUT	C21-C26-C25	5.12	120.58	111.42
48	S	620	LUT	C21-C26-C25	5.12	120.58	111.42
31	c1	508	CLA	O2A-C1-C2	5.11	122.08	108.64
31	S1	610	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	c1	510	CLA	O2D-CGD-CBD	5.11	120.35	111.27
33	C1	516	BCR	C33-C5-C6	-5.11	118.79	124.53
31	b1	617	CLA	O2A-C1-C2	5.11	122.06	108.64
31	R	609	CLA	O2A-C1-C2	5.11	122.06	108.64
31	y1	604	CLA	O2A-C1-C2	5.11	122.06	108.64

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S1	611	CLA	CMD-C2D-C1D	5.11	133.71	124.71
31	n	613	CLA	O2D-CGD-CBD	5.11	120.34	111.27
48	g1	621	LUT	C21-C26-C27	5.10	119.15	112.70
31	S	611	CLA	CMD-C2D-C1D	5.10	133.71	124.71
31	c1	505	CLA	CMD-C2D-C1D	5.10	133.70	124.71
31	A	406	CLA	O2A-C1-C2	5.10	122.03	108.64
31	Y	613	CLA	CMD-C2D-C1D	5.10	133.70	124.71
31	r1	610	CLA	CMD-C2D-C1D	5.10	133.70	124.71
31	C	506	CLA	O2A-C1-C2	5.10	122.03	108.64
31	A	405	CLA	O2A-C1-C2	5.10	122.03	108.64
31	R	608	CLA	O2A-C1-C2	5.09	122.03	108.64
31	C	512	CLA	O2D-CGD-CBD	5.09	120.32	111.27
31	g	603	CLA	O2A-C1-C2	5.09	122.02	108.64
31	c	503	CLA	O2D-CGD-CBD	5.09	120.31	111.27
31	s	613	CLA	CMD-C2D-C1D	5.09	133.69	124.71
31	y	612	CLA	O2A-C1-C2	5.09	122.01	108.64
31	S1	610	CLA	O2A-C1-C2	5.09	122.01	108.64
31	b	616	CLA	O2D-CGD-CBD	5.09	120.31	111.27
31	C	511	CLA	O2D-CGD-CBD	5.09	120.31	111.27
31	B1	616	CLA	O2A-C1-C2	5.09	122.00	108.64
31	S	617	CLA	CMD-C2D-C1D	5.09	133.68	124.71
31	Y1	610	CLA	CMD-C2D-C1D	5.08	133.67	124.71
31	C	509	CLA	O2D-CGD-CBD	5.08	120.30	111.27
31	Y1	610	CLA	O2D-CGD-CBD	5.08	120.30	111.27
31	B1	616	CLA	O2D-CGD-CBD	5.08	120.30	111.27
31	C1	513	CLA	O2D-CGD-CBD	5.08	120.30	111.27
31	S	602	CLA	O2A-C1-C2	5.08	121.98	108.64
31	R1	610	CLA	O2D-CGD-CBD	5.08	120.29	111.27
31	S	610	CLA	O2A-C1-C2	5.08	121.98	108.64
31	r	610	CLA	O2A-C1-C2	5.08	121.98	108.64
31	N	603	CLA	O2A-C1-C2	5.08	121.98	108.64
48	n	620	LUT	C21-C26-C27	5.08	119.12	112.70
31	B	608	CLA	O2A-C1-C2	5.07	121.97	108.64
31	r	602	CLA	O2A-C1-C2	5.07	121.97	108.64
31	R1	609	CLA	CMD-C2D-C1D	5.07	133.65	124.71
31	Y1	613	CLA	O2A-C1-C2	5.07	121.97	108.64
31	G1	604	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	Y1	608	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	D1	403	CLA	O2A-C1-C2	5.07	121.96	108.64
31	S1	612	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	S1	602	CLA	CMD-C2D-C1D	5.07	133.65	124.71
31	B1	612	CLA	O2D-CGD-CBD	5.06	120.26	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	614	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	R1	610	CLA	CMD-C2D-C1D	5.06	133.63	124.71
31	C	501	CLA	O2A-C1-C2	5.06	121.94	108.64
31	n	612	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	g1	603	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	c	508	CLA	CMD-C2D-C1D	5.06	133.63	124.71
50	Y1	623	NEX	C2-C1-C6	5.06	114.13	109.21
31	s1	609	CLA	CMD-C2D-C1D	5.06	133.63	124.71
31	y1	602	CLA	O2A-C1-C2	5.06	121.93	108.64
31	y1	614	CLA	O2D-CGD-CBD	5.06	120.25	111.27
48	G	621	LUT	C21-C26-C25	5.06	120.47	111.42
41	N	624	LHG	O7-C7-C8	5.06	122.40	111.50
31	S	604	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	R1	604	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	n1	611	CLA	O2D-CGD-CBD	5.05	120.25	111.27
50	Y	623	NEX	C2-C1-C6	5.05	114.12	109.21
49	N	622	XAT	C15-C14-C13	-5.05	120.10	127.31
31	N	602	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	R1	612	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	N1	614	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	B	612	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	Y	604	CLA	O2A-C1-C2	5.05	121.90	108.64
31	N1	613	CLA	O2D-CGD-CBD	5.04	120.23	111.27
31	B1	617	CLA	O2D-CGD-CBD	5.04	120.23	111.27
31	b1	612	CLA	O2D-CGD-CBD	5.04	120.23	111.27
31	y	612	CLA	CMD-C2D-C1D	5.04	133.60	124.71
49	y1	622	XAT	C31-C30-C29	-5.04	120.12	127.31
31	R1	610	CLA	O2A-C1-C2	5.04	121.88	108.64
48	g1	620	LUT	C21-C26-C27	5.04	119.07	112.70
31	C	507	CLA	O2D-CGD-CBD	5.04	120.22	111.27
31	a	410	CLA	O2A-C1-C2	5.04	121.87	108.64
31	S1	605	CLA	O2D-CGD-CBD	5.03	120.22	111.27
37	B	620	C7Z	C38-C25-C26	-5.03	118.88	124.53
49	g1	622	XAT	C15-C14-C13	-5.03	120.13	127.31
31	r1	603	CLA	O2D-CGD-CBD	5.03	120.21	111.27
33	C1	517	BCR	C15-C14-C13	-5.03	120.13	127.31
31	S	617	CLA	O2D-CGD-CBD	5.03	120.21	111.27
31	b1	611	CLA	O2A-C1-C2	5.03	121.86	108.64
31	r1	612	CLA	O2D-CGD-CBD	5.03	120.21	111.27
37	b	620	C7Z	C18-C5-C6	-5.03	118.88	124.53
31	b1	612	CLA	CMD-C2D-C1D	5.03	133.58	124.71
31	d	403	CLA	O2A-C1-C2	5.03	121.85	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	509	CLA	O2D-CGD-CBD	5.03	120.20	111.27
48	N	620	LUT	C35-C34-C33	-5.03	120.14	127.31
31	B1	609	CLA	CMD-C2D-C1D	5.03	133.57	124.71
31	d	403	CLA	CMD-C2D-C1D	5.03	133.57	124.71
31	Y	608	CLA	O2A-C1-C2	5.03	121.84	108.64
31	G	613	CLA	O2A-C1-C2	5.02	121.84	108.64
31	G1	611	CLA	O2A-C1-C2	5.02	121.84	108.64
31	C	505	CLA	CMD-C2D-C1D	5.02	133.57	124.71
31	C	505	CLA	O2A-C1-C2	5.02	121.84	108.64
37	b	620	C7Z	C35-C34-C33	-5.02	120.14	127.31
31	s	614	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	B	602	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	r1	609	CLA	CMD-C2D-C1D	5.02	133.56	124.71
48	Y1	620	LUT	C15-C14-C13	-5.02	120.14	127.31
31	s1	610	CLA	O2A-C1-C2	5.02	121.83	108.64
31	C	510	CLA	O2A-C1-C2	5.02	121.83	108.64
31	b1	615	CLA	O2A-C1-C2	5.02	121.82	108.64
31	B1	602	CLA	O2D-CGD-CBD	5.02	120.18	111.27
31	c	511	CLA	O2D-CGD-CBD	5.01	120.18	111.27
31	S1	610	CLA	CMD-C2D-C1D	5.01	133.55	124.71
31	n1	612	CLA	O2D-CGD-CBD	5.01	120.18	111.27
48	s	620	LUT	C35-C34-C33	-5.01	120.16	127.31
31	y	613	CLA	O2D-CGD-CBD	5.01	120.17	111.27
31	b1	604	CLA	O2A-C1-C2	5.01	121.80	108.64
31	C	512	CLA	CMD-C2D-C1D	5.01	133.54	124.71
31	s	612	CLA	O2D-CGD-CBD	5.01	120.17	111.27
31	s	617	CLA	O2D-CGD-CBD	5.01	120.17	111.27
31	g1	611	CLA	O2D-CGD-CBD	5.01	120.17	111.27
31	c	508	CLA	O2A-C1-C2	5.01	121.80	108.64
31	r1	603	CLA	CMD-C2D-C1D	5.01	133.54	124.71
31	B1	609	CLA	O2A-C1-C2	5.01	121.79	108.64
31	S1	617	CLA	O2D-CGD-CBD	5.01	120.16	111.27
48	n	621	LUT	C21-C26-C25	5.00	120.38	111.42
31	B	604	CLA	O2D-CGD-CBD	5.00	120.16	111.27
31	Y	608	CLA	O2D-CGD-CBD	5.00	120.16	111.27
31	c	508	CLA	O2D-CGD-CBD	5.00	120.15	111.27
31	S	614	CLA	CMD-C2D-C1D	5.00	133.52	124.71
35	c	521	LMG	O7-C10-C11	4.99	122.27	111.50
31	Y1	611	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	G	612	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	b	603	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	b	604	CLA	O2D-CGD-CBD	4.99	120.13	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	614	CLA	CMD-C2D-C1D	4.99	133.50	124.71
31	S1	617	CLA	CMD-C2D-C1D	4.99	133.50	124.71
31	C1	506	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	S1	611	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	b1	617	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	b1	610	CLA	O2A-C1-C2	4.98	121.72	108.64
31	g	603	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	N1	602	CLA	O2D-CGD-CBD	4.98	120.11	111.27
49	N	622	XAT	C31-C30-C29	-4.98	120.21	127.31
31	N1	612	CLA	O2D-CGD-CBD	4.98	120.11	111.27
31	s	604	CLA	O2A-C1-C2	4.98	121.71	108.64
31	C1	501	CLA	O2D-CGD-CBD	4.97	120.11	111.27
31	b	614	CLA	O2A-C1-C2	4.97	121.71	108.64
31	c	504	CLA	O2D-CGD-CBD	4.97	120.11	111.27
31	n	603	CLA	O2D-CGD-CBD	4.97	120.11	111.27
31	R	612	CLA	O2D-CGD-CBD	4.97	120.10	111.27
31	d1	402	CLA	CMD-C2D-C1D	4.97	133.47	124.71
31	c1	509	CLA	O2D-CGD-CBD	4.97	120.10	111.27
31	A1	405	CLA	CAC-C3C-C2C	4.96	136.02	127.53
31	y1	603	CLA	O2A-C1-C2	4.96	121.68	108.64
48	r	620	LUT	C7-C8-C9	-4.96	118.74	126.23
31	R1	603	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	N	610	CLA	O2A-C1-C2	4.96	121.67	108.64
31	b1	602	CLA	O2A-C1-C2	4.96	121.67	108.64
48	g	620	LUT	C35-C34-C33	-4.96	120.23	127.31
50	s1	623	NEX	C38-C25-C24	4.96	119.86	114.28
31	C1	506	CLA	O2A-C1-C2	4.96	121.66	108.64
31	B	616	CLA	O2A-C1-C2	4.95	121.65	108.64
31	s1	603	CLA	O2A-C1-C2	4.95	121.64	108.64
31	s1	611	CLA	O2A-C1-C2	4.95	121.64	108.64
31	c1	503	CLA	O2A-C1-C2	4.95	121.63	108.64
31	r1	604	CLA	O2D-CGD-CBD	4.95	120.06	111.27
31	b	606	CLA	O2D-CGD-CBD	4.94	120.05	111.27
31	C1	502	CLA	O2D-CGD-CBD	4.94	120.05	111.27
31	a1	406	CLA	O2A-C1-C2	4.94	121.62	108.64
50	g1	623	NEX	C2-C1-C6	4.94	114.01	109.21
49	G	622	XAT	C15-C14-C13	-4.94	120.26	127.31
46	h1	101	RRX	C24-C25-C26	-4.94	109.50	121.46
49	y	622	XAT	C15-C14-C13	-4.94	120.26	127.31
31	N	602	CLA	O2A-C1-C2	4.94	121.61	108.64
31	c1	502	CLA	O2D-CGD-CBD	4.93	120.04	111.27
31	b1	616	CLA	O2D-CGD-CBD	4.93	120.04	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	511	CLA	O2A-C1-C2	4.93	121.60	108.64
31	B1	606	CLA	O2D-CGD-CBD	4.93	120.03	111.27
31	S	603	CLA	O2D-CGD-CBD	4.93	120.03	111.27
31	A1	410	CLA	O2D-CGD-CBD	4.93	120.03	111.27
48	s	620	LUT	C11-C10-C9	-4.93	120.28	127.31
31	d1	402	CLA	O2A-C1-C2	4.93	121.59	108.64
31	Y1	612	CLA	O2A-C1-C2	4.93	121.59	108.64
31	A1	405	CLA	O2A-C1-C2	4.93	121.58	108.64
46	H1	101	RRX	C7-C8-C9	-4.93	118.79	126.23
31	c	503	CLA	O2A-C1-C2	4.92	121.58	108.64
31	S	603	CLA	O2A-C1-C2	4.92	121.58	108.64
31	y1	608	CLA	O2A-C1-C2	4.92	121.58	108.64
48	S1	621	LUT	C21-C26-C25	4.92	120.24	111.42
31	B1	612	CLA	CMD-C2D-C1D	4.92	133.39	124.71
31	y	611	CLA	O2A-C1-C2	4.92	121.57	108.64
49	y1	622	XAT	C15-C14-C13	-4.92	120.29	127.31
31	c	509	CLA	O2D-CGD-CBD	4.92	120.01	111.27
31	C1	502	CLA	O2A-C1-C2	4.92	121.56	108.64
31	R1	603	CLA	O2A-C1-C2	4.92	121.56	108.64
48	S	621	LUT	C21-C26-C25	4.91	120.22	111.42
31	B1	617	CLA	O2A-C1-C2	4.91	121.55	108.64
31	r	608	CLA	O2D-CGD-CBD	4.91	119.99	111.27
31	y1	613	CLA	O2D-CGD-CBD	4.91	119.99	111.27
33	D1	404	BCR	C19-C18-C17	4.91	126.47	118.94
48	g	620	LUT	C21-C26-C27	4.91	118.90	112.70
49	R	621	XAT	C38-C25-C24	4.91	119.80	114.28
48	r	620	LUT	C15-C14-C13	-4.90	120.31	127.31
31	C	503	CLA	O2D-CGD-CBD	4.90	119.98	111.27
44	d	405	PL9	C7-C3-C4	4.90	120.86	116.88
31	Y1	613	CLA	O2D-CGD-CBD	4.90	119.97	111.27
31	g	613	CLA	O2A-C1-C2	4.90	121.50	108.64
31	r	611	CLA	O2D-CGD-CBD	4.90	119.97	111.27
31	N	612	CLA	O2D-CGD-CBD	4.89	119.97	111.27
31	N	611	CLA	O2A-C1-C2	4.89	120.42	108.97
31	b	614	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	B1	611	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	g	604	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	b	602	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	G1	614	CLA	O2D-CGD-CBD	4.89	119.96	111.27
48	n	620	LUT	C35-C34-C33	-4.89	120.33	127.31
49	N	622	XAT	C38-C25-C24	4.89	119.78	114.28
31	b1	611	CLA	CMD-C2D-C1D	4.89	133.33	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	609	CLA	O2D-CGD-CBD	4.89	119.96	111.27
57	y1	627	PTY	O7-C8-C11	4.89	120.08	111.09
31	B	617	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	R	603	CLA	O2A-C1-C2	4.89	121.47	108.64
31	N1	611	CLA	O2D-CGD-CBD	4.88	119.94	111.27
31	B1	608	CLA	O2D-CGD-CBD	4.88	119.94	111.27
37	b	620	C7Z	C15-C14-C13	-4.88	120.35	127.31
31	b1	615	CLA	O2D-CGD-CBD	4.88	119.94	111.27
31	r1	610	CLA	O2D-CGD-CBD	4.88	119.94	111.27
50	n1	623	NEX	C17-C1-C6	-4.88	106.11	110.47
31	d1	403	CLA	O2D-CGD-CBD	4.87	119.93	111.27
31	b	616	CLA	O2A-C1-C2	4.87	121.44	108.64
31	Y1	602	CLA	O2D-CGD-CBD	4.87	119.93	111.27
31	b1	610	CLA	O2D-CGD-CBD	4.87	119.93	111.27
50	r	623	NEX	C38-C25-C24	4.87	119.76	114.28
48	G1	621	LUT	C35-C34-C33	-4.87	120.36	127.31
31	C1	513	CLA	O2A-C1-C2	4.87	121.43	108.64
31	s	603	CLA	O2D-CGD-CBD	4.87	119.92	111.27
31	S1	611	CLA	O2A-C1-C2	4.86	121.42	108.64
31	B	613	CLA	O2D-CGD-CBD	4.86	119.91	111.27
31	B1	611	CLA	O2A-C1-C2	4.86	121.41	108.64
48	R	620	LUT	C11-C10-C9	-4.86	120.37	127.31
37	B1	620	C7Z	C18-C5-C6	-4.86	119.07	124.53
48	n1	620	LUT	C21-C26-C25	4.86	120.12	111.42
31	D	402	CLA	O2D-CGD-CBD	4.86	119.90	111.27
31	N1	610	CLA	O2A-C1-C2	4.86	121.39	108.64
31	B1	603	CLA	O2A-C1-C2	4.85	121.39	108.64
31	b1	602	CLA	O2D-CGD-CBD	4.85	119.89	111.27
31	s	611	CLA	O2A-C1-C2	4.85	121.39	108.64
31	S	614	CLA	O2A-C1-C2	4.85	121.38	108.64
40	b1	623	DGD	O2G-C1B-C2B	4.85	121.95	111.50
31	N	612	CLA	CMD-C2D-C1D	4.85	133.25	124.71
31	b	617	CLA	O2D-CGD-CBD	4.84	119.87	111.27
31	B1	613	CLA	O2A-C1-C2	4.84	121.35	108.64
31	Y	612	CLA	CMD-C2D-C1D	4.84	133.24	124.71
31	B	610	CLA	CMD-C2D-C1D	4.84	133.24	124.71
31	b1	606	CLA	O2A-C1-C2	4.84	121.34	108.64
31	A1	410	CLA	O2A-C1-C2	4.84	121.34	108.64
31	N1	602	CLA	O2A-C1-C2	4.84	121.34	108.64
31	Y1	611	CLA	O2A-C1-C2	4.83	121.34	108.64
31	c1	502	CLA	O2A-C1-C2	4.83	121.34	108.64
31	A1	406	CLA	O2A-C1-C2	4.83	121.34	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	609	CLA	O2A-C1-C2	4.83	121.33	108.64
31	c	505	CLA	CMD-C2D-C1D	4.83	133.22	124.71
31	Y	613	CLA	O2D-CGD-CBD	4.83	119.85	111.27
31	G1	602	CLA	O2D-CGD-CBD	4.83	119.85	111.27
31	B1	607	CLA	O2A-C1-C2	4.83	121.32	108.64
31	S	602	CLA	O2D-CGD-CBD	4.83	119.84	111.27
31	G1	613	CLA	O2D-CGD-CBD	4.83	119.84	111.27
31	G1	610	CLA	O2D-CGD-CBD	4.82	119.83	111.27
49	n	622	XAT	C7-C8-C9	-4.82	118.05	125.53
31	n1	614	CLA	O2D-CGD-CBD	4.82	119.83	111.27
35	b	622	LMG	O7-C10-C11	4.82	121.89	111.50
37	b1	620	C7Z	C11-C10-C9	-4.82	120.43	127.31
31	C1	512	CLA	O2D-CGD-CBD	4.82	119.83	111.27
57	Y1	627	PTY	O7-C8-C11	4.82	119.95	111.09
31	G	603	CLA	O2A-C1-C2	4.81	121.28	108.64
48	s	621	LUT	C21-C26-C27	4.81	118.78	112.70
31	N1	602	CLA	CMD-C2D-C1D	4.81	133.19	124.71
31	s1	604	CLA	O2A-C1-C2	4.81	121.27	108.64
31	g1	614	CLA	O2D-CGD-CBD	4.81	119.81	111.27
33	c	514	BCR	C15-C14-C13	-4.81	120.45	127.31
31	c1	508	CLA	O2D-CGD-CBD	4.81	119.81	111.27
31	g1	610	CLA	O2A-C1-C2	4.80	121.26	108.64
46	h1	101	RRX	C15-C16-C17	-4.80	113.64	123.47
31	Y1	614	CLA	O2A-C1-C2	4.79	121.23	108.64
50	g1	623	NEX	C38-C25-C24	4.79	119.67	114.28
31	R1	608	CLA	O2A-C1-C2	4.79	121.22	108.64
48	r1	620	LUT	C15-C14-C13	-4.79	120.48	127.31
48	y1	621	LUT	C22-C23-C24	-4.78	106.30	111.74
31	b	608	CLA	O2D-CGD-CBD	4.78	119.76	111.27
31	s1	602	CLA	O2A-C1-C2	4.78	121.19	108.64
31	b	606	CLA	O2A-C1-C2	4.78	121.19	108.64
31	B	611	CLA	CMD-C2D-C1D	4.77	133.13	124.71
31	c1	507	CLA	O2D-CGD-CBD	4.77	119.75	111.27
31	C1	507	CLA	O2D-CGD-CBD	4.77	119.75	111.27
48	g1	620	LUT	C21-C26-C25	4.77	119.96	111.42
31	B	614	CLA	O2A-C1-C2	4.77	121.17	108.64
31	b	609	CLA	O2A-C1-C2	4.77	121.17	108.64
31	c	507	CLA	O2A-C1-C2	4.77	121.16	108.64
31	b	615	CLA	O2D-CGD-CBD	4.76	119.73	111.27
31	C	503	CLA	O2A-C1-C2	4.76	121.14	108.64
31	d1	402	CLA	O2D-CGD-CBD	4.76	119.72	111.27
31	a	406	CLA	O2A-C1-C2	4.75	121.12	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Y1	621	LUT	C21-C26-C27	4.75	118.70	112.70
31	c	509	CLA	O2A-C1-C2	4.75	121.11	108.64
37	b1	620	C7Z	C38-C25-C26	-4.75	119.20	124.53
31	R1	609	CLA	O2D-CGD-CBD	4.75	119.70	111.27
31	D1	402	CLA	O2D-CGD-CBD	4.75	119.70	111.27
49	y	622	XAT	C18-C5-C4	4.74	119.61	114.28
31	b1	608	CLA	O2D-CGD-CBD	4.74	119.69	111.27
31	g	613	CLA	O2D-CGD-CBD	4.74	119.68	111.27
31	B1	607	CLA	O2D-CGD-CBD	4.73	119.68	111.27
31	B	602	CLA	O2A-C1-C2	4.73	121.08	108.64
31	c	502	CLA	O2D-CGD-CBD	4.73	119.68	111.27
31	B1	605	CLA	O2D-CGD-CBD	4.73	119.68	111.27
31	R	608	CLA	O2D-CGD-CBD	4.73	119.67	111.27
31	c1	504	CLA	O2D-CGD-CBD	4.73	119.67	111.27
31	g	610	CLA	O2D-CGD-CBD	4.73	119.67	111.27
31	G1	603	CLA	O2D-CGD-CBD	4.73	119.67	111.27
31	n1	613	CLA	O2D-CGD-CBD	4.72	119.66	111.27
31	N	613	CLA	O2D-CGD-CBD	4.72	119.66	111.27
31	a1	410	CLA	O2A-C1-C2	4.71	121.02	108.64
50	y	623	NEX	C31-C30-C29	4.71	134.03	127.31
31	c	511	CLA	O2A-C1-C2	4.71	121.00	108.64
49	y1	622	XAT	C7-C8-C9	-4.70	118.23	125.53
50	R1	622	NEX	C38-C25-C24	4.70	119.57	114.28
50	r	623	NEX	C17-C1-C6	-4.70	106.27	110.47
31	c1	510	CLA	O2A-C1-C2	4.70	120.98	108.64
48	s	620	LUT	C22-C23-C24	-4.70	106.40	111.74
31	r	603	CLA	O2D-CGD-CBD	4.69	119.61	111.27
31	Y1	604	CLA	O2A-C1-C2	4.69	120.97	108.64
31	S	609	CLA	O2A-C1-C2	4.69	120.96	108.64
31	B	611	CLA	O2D-CGD-CBD	4.69	119.60	111.27
49	G1	622	XAT	C15-C14-C13	-4.69	120.62	127.31
31	C1	511	CLA	O2D-CGD-CBD	4.69	119.60	111.27
31	C	507	CLA	O2A-C1-C2	4.69	120.95	108.64
50	g	623	NEX	C38-C25-C24	4.69	119.55	114.28
31	S	612	CLA	CMD-C2D-C1D	4.68	132.97	124.71
48	Y	620	LUT	C15-C14-C13	-4.68	120.63	127.31
37	B	620	C7Z	C18-C5-C6	-4.68	119.27	124.53
31	Y	612	CLA	O2A-C1-C2	4.68	120.92	108.64
31	s	604	CLA	O2D-CGD-CBD	4.68	119.58	111.27
31	S	610	CLA	O2D-CGD-CBD	4.68	119.58	111.27
31	B1	602	CLA	O2A-C1-C2	4.67	120.92	108.64
37	b	620	C7Z	C38-C25-C26	-4.67	119.28	124.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Y1	622	XAT	C31-C30-C29	-4.67	120.64	127.31
41	C1	525	LHG	O7-C7-C8	4.67	121.57	111.50
49	R	621	XAT	C7-C8-C9	-4.67	118.28	125.53
37	B1	620	C7Z	C11-C10-C9	-4.67	120.65	127.31
37	B1	620	C7Z	C22-C23-C24	4.67	116.69	110.30
31	N	610	CLA	CMD-C2D-C1D	4.66	132.93	124.71
50	n1	623	NEX	C31-C30-C29	4.66	133.97	127.31
50	s	623	NEX	C38-C25-C24	4.66	119.53	114.28
31	N1	603	CLA	O2D-CGD-CBD	4.66	119.56	111.27
46	H1	101	RRX	C11-C10-C9	-4.66	120.66	127.31
31	R	609	CLA	O2D-CGD-CBD	4.66	119.55	111.27
31	S1	614	CLA	O2A-C1-C2	4.66	120.89	108.64
31	y	608	CLA	O2D-CGD-CBD	4.66	119.55	111.27
31	r	609	CLA	O2D-CGD-CBD	4.66	119.55	111.27
31	Y	613	CLA	O2A-C1-C2	4.66	120.88	108.64
31	g1	610	CLA	O2D-CGD-CBD	4.65	119.54	111.27
31	B	612	CLA	O2A-C1-C2	4.65	120.86	108.64
48	s1	620	LUT	C7-C8-C9	-4.65	119.21	126.23
31	B	608	CLA	O2D-CGD-CBD	4.65	119.53	111.27
31	S	604	CLA	O2A-C1-C2	4.65	120.86	108.64
50	Y1	623	NEX	C38-C25-C24	4.65	119.51	114.28
31	n1	610	CLA	O2A-C1-C2	4.65	120.85	108.64
31	b1	605	CLA	C2C-C1C-NC	4.65	114.33	109.97
31	C	505	CLA	O2D-CGD-CBD	4.65	119.53	111.27
31	B	610	CLA	O2A-C1-C2	4.64	120.83	108.64
31	y	603	CLA	O2A-C1-C2	4.64	120.83	108.64
48	r1	620	LUT	C7-C8-C9	-4.64	119.23	126.23
31	S	611	CLA	O2A-C1-C2	4.64	120.82	108.64
31	b1	609	CLA	O2A-C1-C2	4.64	120.82	108.64
31	C1	508	CLA	CMD-C2D-C1D	4.64	132.88	124.71
31	r1	609	CLA	O2D-CGD-CBD	4.63	119.50	111.27
31	s1	617	CLA	O2A-C1-C2	4.63	120.81	108.64
31	n	610	CLA	O2D-CGD-CBD	4.63	119.50	111.27
31	b1	604	CLA	O2D-CGD-CBD	4.63	119.50	111.27
48	S	621	LUT	C35-C34-C33	-4.63	120.70	127.31
31	y1	614	CLA	O2A-C1-C2	4.63	120.80	108.64
31	d	402	CLA	O2D-CGD-CBD	4.63	119.49	111.27
41	g	624	LHG	O7-C7-C8	4.63	121.47	111.50
31	S1	609	CLA	O2A-C1-C2	4.63	120.79	108.64
31	B1	604	CLA	O2D-CGD-CBD	4.63	119.49	111.27
31	C1	510	CLA	O2D-CGD-CBD	4.62	119.48	111.27
31	Y	603	CLA	O2A-C1-C2	4.62	120.78	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	608	CLA	O2A-C1-C2	4.62	120.77	108.64
48	g	620	LUT	C7-C8-C9	-4.62	119.26	126.23
31	y1	610	CLA	O2D-CGD-CBD	4.62	119.47	111.27
35	W1	201	LMG	O7-C10-C11	4.62	121.45	111.50
31	Y	611	CLA	O2A-C1-C2	4.62	120.77	108.64
48	R	620	LUT	C15-C14-C13	-4.61	120.73	127.31
31	B	606	CLA	O2D-CGD-CBD	4.61	119.46	111.27
31	y	604	CLA	O2D-CGD-CBD	4.61	119.46	111.27
49	N1	622	XAT	C18-C5-C4	4.61	119.47	114.28
31	B1	610	CLA	O2D-CGD-CBD	4.61	119.46	111.27
48	Y	620	LUT	C22-C23-C24	-4.61	106.50	111.74
49	N1	622	XAT	C38-C25-C24	4.61	119.46	114.28
46	H1	101	RRX	C15-C16-C17	-4.60	114.04	123.47
49	G	622	XAT	C18-C5-C4	4.60	119.46	114.28
31	C	512	CLA	O2A-C1-C2	4.60	120.73	108.64
49	g	622	XAT	C31-C30-C29	-4.60	120.74	127.31
49	Y1	622	XAT	C38-C25-C24	4.60	119.46	114.28
31	b	612	CLA	CMD-C2D-C1D	4.60	132.82	124.71
31	Y	602	CLA	CMD-C2D-C1D	4.60	132.82	124.71
31	y1	608	CLA	O2D-CGD-CBD	4.60	119.44	111.27
31	c1	508	CLA	CMD-C2D-C1D	4.59	132.81	124.71
50	Y	623	NEX	C38-C25-C24	4.59	119.45	114.28
31	b1	614	CLA	O2D-CGD-CBD	4.59	119.42	111.27
31	r	610	CLA	O2D-CGD-CBD	4.59	119.42	111.27
48	G	620	LUT	C7-C8-C9	-4.59	119.30	126.23
31	B	613	CLA	O2A-C1-C2	4.59	120.69	108.64
48	r1	620	LUT	C11-C10-C9	-4.59	120.76	127.31
50	r1	622	NEX	C38-C25-C24	4.59	119.44	114.28
31	s1	617	CLA	O2D-CGD-CBD	4.58	119.42	111.27
49	Y1	622	XAT	C18-C5-C4	4.58	119.44	114.28
50	R	622	NEX	C38-C25-C24	4.58	119.44	114.28
31	s	602	CLA	O2D-CGD-CBD	4.58	119.41	111.27
35	A1	413	LMG	O7-C10-C11	4.58	121.38	111.50
31	G1	612	CLA	CMD-C2D-C1D	4.58	132.79	124.71
49	y1	622	XAT	C18-C5-C4	4.58	119.43	114.28
31	C1	510	CLA	O2A-C1-C2	4.58	120.67	108.64
49	R1	621	XAT	C18-C5-C4	4.58	119.43	114.28
31	A1	405	CLA	O2D-CGD-CBD	4.57	119.39	111.27
31	b	605	CLA	O2A-C1-C2	4.57	120.65	108.64
37	b1	620	C7Z	C1-C6-C5	-4.57	116.17	122.61
41	n	624	LHG	O7-C7-C8	4.57	121.35	111.50
49	R1	621	XAT	C38-C25-C24	4.56	119.41	114.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Y	622	XAT	C38-C25-C24	4.56	119.41	114.28
35	B1	622	LMG	O7-C10-C11	4.56	121.33	111.50
31	C	508	CLA	O2D-CGD-CBD	4.56	119.37	111.27
31	B1	614	CLA	O2A-C1-C2	4.56	120.61	108.64
31	g1	613	CLA	O2D-CGD-CBD	4.56	119.36	111.27
31	c	505	CLA	O2D-CGD-CBD	4.55	119.36	111.27
31	Y1	608	CLA	O2A-C1-C2	4.55	120.59	108.64
46	H1	101	RRX	C24-C23-C22	4.55	133.11	126.23
48	S1	621	LUT	C21-C26-C27	4.55	118.45	112.70
31	R1	608	CLA	O2D-CGD-CBD	4.54	119.34	111.27
48	N1	620	LUT	C21-C26-C27	4.54	118.44	112.70
50	y	623	NEX	C2-C1-C6	4.54	113.62	109.21
50	N	623	NEX	C38-C25-C24	4.54	119.39	114.28
31	s1	613	CLA	O2D-CGD-CBD	4.54	119.33	111.27
31	S1	613	CLA	O2D-CGD-CBD	4.53	119.32	111.27
49	G1	622	XAT	C31-C30-C29	-4.53	120.84	127.31
31	y1	613	CLA	O2A-C1-C2	4.53	120.54	108.64
32	A1	409	PHO	CMB-C2B-C3B	4.53	133.15	124.68
46	H1	101	RRX	C24-C25-C26	-4.53	110.50	121.46
50	n	623	NEX	C27-C28-C29	-4.53	118.51	125.53
35	b1	622	LMG	O7-C10-C11	4.52	121.25	111.50
31	g1	604	CLA	O2A-C1-C2	4.52	119.55	108.97
33	C	516	BCR	C33-C5-C6	-4.52	119.45	124.53
49	r	622	XAT	C38-C25-C24	4.52	119.37	114.28
48	s	620	LUT	C15-C14-C13	-4.52	120.86	127.31
31	B	614	CLA	O2D-CGD-CBD	4.52	119.30	111.27
49	n1	622	XAT	C18-C5-C4	4.52	119.36	114.28
50	N1	623	NEX	C38-C25-C24	4.52	119.36	114.28
31	R	612	CLA	O2A-C1-C2	4.52	120.51	108.64
31	G1	602	CLA	CMD-C2D-C1D	4.51	132.67	124.71
48	N	620	LUT	C15-C14-C13	-4.51	120.87	127.31
31	C1	511	CLA	O2A-C1-C2	4.51	120.49	108.64
31	s1	614	CLA	O2A-C1-C2	4.51	120.49	108.64
48	n	620	LUT	C11-C10-C9	-4.51	120.87	127.31
31	c1	505	CLA	O2A-C1-C2	4.51	120.48	108.64
31	R1	602	CLA	O2A-C1-C2	4.50	120.47	108.64
48	S	621	LUT	C21-C26-C27	4.50	118.39	112.70
48	G	620	LUT	C21-C26-C25	4.50	119.48	111.42
48	y	620	LUT	C7-C8-C9	-4.50	119.44	126.23
31	c	513	CLA	CMD-C2D-C1D	4.50	132.64	124.71
49	n	622	XAT	C38-C25-C24	4.49	119.33	114.28
31	B1	613	CLA	CMD-C2D-C1D	4.48	132.62	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	y1	623	NEX	C2-C1-C6	4.48	113.57	109.21
50	S1	623	NEX	C38-C25-C24	4.48	119.32	114.28
31	n1	610	CLA	O2D-CGD-CBD	4.48	119.23	111.27
49	r1	621	XAT	C18-C5-C4	4.48	119.32	114.28
31	s	603	CLA	O2A-C1-C2	4.48	120.40	108.64
31	s	617	CLA	O2A-C1-C2	4.48	120.40	108.64
48	N1	621	LUT	C35-C34-C33	-4.48	120.92	127.31
37	B1	620	C7Z	C7-C8-C9	-4.48	119.47	126.23
46	h1	101	RRX	C7-C8-C9	4.47	132.99	126.23
31	A1	407	CLA	O2A-C1-C2	4.47	120.38	108.64
31	B1	615	CLA	O2A-C1-C2	4.47	120.38	108.64
31	s	610	CLA	O2D-CGD-CBD	4.47	119.20	111.27
31	B1	615	CLA	O2D-CGD-CBD	4.46	119.20	111.27
49	N	622	XAT	C18-C5-C4	4.46	119.30	114.28
31	A	407	CLA	O2D-CGD-CBD	4.46	119.20	111.27
31	y1	611	CLA	O2D-CGD-CBD	4.46	119.19	111.27
48	Y1	621	LUT	C22-C23-C24	-4.46	106.67	111.74
49	g	622	XAT	C18-C5-C4	4.45	119.29	114.28
48	y1	620	LUT	C21-C26-C27	4.45	118.33	112.70
48	s	621	LUT	C21-C26-C25	4.45	119.39	111.42
31	C1	508	CLA	O2D-CGD-CBD	4.45	119.17	111.27
48	n1	621	LUT	C35-C34-C33	-4.45	120.96	127.31
48	s	620	LUT	C31-C30-C29	-4.45	120.97	127.31
31	C1	504	CLA	O2D-CGD-CBD	4.44	119.16	111.27
31	r1	602	CLA	O2A-C1-C2	4.44	120.30	108.64
48	r1	620	LUT	C21-C26-C25	4.44	119.37	111.42
31	c	509	CLA	C2C-C1C-NC	4.44	114.13	109.97
50	S	622	NEX	C38-C25-C24	4.44	119.27	114.28
49	g1	622	XAT	C31-C30-C29	-4.43	120.98	127.31
48	g	621	LUT	C11-C10-C9	-4.43	120.98	127.31
48	s1	620	LUT	C21-C26-C27	4.43	118.30	112.70
31	b	607	CLA	O2A-C1-C2	4.42	120.26	108.64
41	d	408	LHG	O7-C7-C8	4.42	121.03	111.50
31	b1	614	CLA	O2A-C1-C2	4.42	120.25	108.64
41	D	409	LHG	O7-C7-C8	4.41	121.02	111.50
41	N1	624	LHG	O7-C7-C8	4.41	121.01	111.50
48	n	620	LUT	C31-C30-C29	-4.41	121.02	127.31
37	B	620	C7Z	C35-C34-C33	-4.41	121.02	127.31
37	b1	620	C7Z	C27-C28-C29	-4.40	119.58	126.23
35	c1	521	LMG	O7-C10-C11	4.40	120.99	111.50
48	Y	621	LUT	C35-C34-C33	-4.40	121.03	127.31
48	Y	621	LUT	C21-C26-C27	4.40	118.26	112.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	R	622	NEX	C17-C1-C6	-4.40	106.53	110.47
50	G	623	NEX	C38-C25-C24	4.40	119.23	114.28
31	y	613	CLA	O2A-C1-C2	4.40	120.20	108.64
48	y	620	LUT	C11-C10-C9	-4.40	121.03	127.31
31	y	602	CLA	CMD-C2D-C1D	4.40	132.46	124.71
31	A	405	CLA	O2D-CGD-CBD	4.39	119.08	111.27
48	N	621	LUT	C21-C26-C27	4.39	118.25	112.70
41	S1	624	LHG	O7-C7-C8	4.38	120.94	111.50
49	G	622	XAT	C31-C30-C29	-4.38	121.06	127.31
31	A1	406	CLA	O2D-CGD-CBD	4.38	119.05	111.27
41	d	410	LHG	O7-C7-C8	4.38	120.93	111.50
41	g1	624	LHG	O7-C7-C8	4.38	120.93	111.50
48	s1	620	LUT	C11-C10-C9	-4.37	121.07	127.31
33	d	404	BCR	C1-C6-C5	-4.37	116.45	122.61
48	n1	621	LUT	C22-C23-C24	-4.37	106.76	111.74
31	Y	611	CLA	O2D-CGD-CBD	4.37	119.03	111.27
40	C	519	DGD	O2G-C1B-C2B	4.37	120.91	111.50
31	c	502	CLA	C1-C2-C3	-4.37	118.49	126.04
49	r1	621	XAT	C31-C30-C29	-4.37	121.08	127.31
49	G	622	XAT	C38-C25-C24	4.37	119.19	114.28
31	a	405	CLA	O2D-CGD-CBD	4.36	119.02	111.27
31	C	509	CLA	O2A-C1-C2	4.36	120.09	108.64
47	g	606	CHL	CHD-C1D-ND	-4.35	120.45	124.45
41	S	624	LHG	O7-C7-C8	4.35	120.88	111.50
48	S1	621	LUT	C35-C34-C33	-4.35	121.10	127.31
31	B	607	CLA	O2A-C1-C2	4.35	120.06	108.64
31	c1	512	CLA	CMD-C2D-C1D	4.35	132.37	124.71
48	G	620	LUT	C11-C10-C9	-4.35	121.11	127.31
50	S1	623	NEX	C2-C1-C6	4.34	113.43	109.21
48	R	620	LUT	C31-C32-C33	-4.34	114.22	126.42
48	N	621	LUT	C11-C10-C9	-4.34	121.11	127.31
48	Y1	621	LUT	C7-C8-C9	-4.34	119.68	126.23
48	n	621	LUT	C22-C23-C24	-4.34	106.80	111.74
48	N	621	LUT	C7-C8-C9	-4.34	119.68	126.23
31	a	406	CLA	O2D-CGD-CBD	4.34	118.97	111.27
37	B1	620	C7Z	C35-C34-C33	-4.34	121.12	127.31
49	g1	622	XAT	C18-C5-C4	4.33	119.15	114.28
41	G	630	LHG	O7-C7-C8	4.33	120.83	111.50
33	C1	514	BCR	C15-C14-C13	-4.33	121.13	127.31
35	a	413	LMG	O7-C10-C11	4.33	120.83	111.50
31	B	617	CLA	CMD-C2D-C1D	4.33	132.34	124.71
40	C	523	DGD	O2G-C1B-C2B	4.32	120.82	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	r1	626	ERG	C18-C13-C12	-4.32	103.76	110.59
48	R	620	LUT	C21-C26-C25	4.32	119.15	111.42
41	d1	410	LHG	O7-C7-C8	4.32	120.81	111.50
41	D1	409	LHG	O7-C7-C8	4.31	120.79	111.50
48	y	620	LUT	C21-C26-C27	4.31	118.15	112.70
48	Y	620	LUT	C21-C26-C27	4.29	118.13	112.70
31	b	609	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
52	i	101	3PH	O21-C21-C22	4.29	120.75	111.50
48	R1	620	LUT	C15-C14-C13	-4.29	121.19	127.31
48	g1	620	LUT	C35-C34-C33	-4.29	121.19	127.31
31	a1	405	CLA	O2D-CGD-CBD	4.29	118.89	111.27
49	g	622	XAT	C38-C25-C24	4.29	119.10	114.28
33	c1	515	BCR	C34-C9-C10	-4.29	116.92	122.92
31	b1	613	CLA	O2A-C1-C2	4.29	119.90	108.64
48	G1	620	LUT	C35-C34-C33	-4.29	121.19	127.31
41	D1	408	LHG	O7-C7-C8	4.28	120.73	111.50
31	c1	506	CLA	O2A-C1-C2	4.28	119.88	108.64
49	G1	622	XAT	C18-C5-C4	4.28	119.09	114.28
31	C1	505	CLA	O2D-CGD-CBD	4.28	118.87	111.27
49	y1	622	XAT	C36-C21-C26	4.27	121.58	110.05
48	s1	621	LUT	C7-C8-C9	-4.27	119.78	126.23
31	s1	614	CLA	O2D-CGD-CBD	4.27	118.86	111.27
33	D	404	BCR	C19-C18-C17	4.27	125.50	118.94
48	n	620	LUT	C21-C26-C25	4.27	119.06	111.42
40	c	520	DGD	O2G-C1B-C2B	4.26	120.69	111.50
48	S1	620	LUT	C21-C26-C25	4.26	119.05	111.42
48	S1	620	LUT	C7-C8-C9	-4.26	119.80	126.23
48	G1	620	LUT	C15-C14-C13	-4.26	121.23	127.31
48	y	621	LUT	C7-C8-C9	-4.26	119.80	126.23
35	w1	201	LMG	O7-C10-C11	4.26	120.67	111.50
50	r	623	NEX	C2-C1-C6	4.25	113.34	109.21
46	H	101	RRX	C30-C25-C26	-4.25	116.63	122.61
31	b	604	CLA	O2A-C1-C2	4.25	119.80	108.64
37	B1	620	C7Z	C21-C26-C25	-4.24	116.64	122.61
31	C1	503	CLA	O2A-C1-C2	4.24	119.77	108.64
48	g	621	LUT	C7-C8-C9	-4.24	119.83	126.23
48	S	620	LUT	C35-C34-C33	-4.24	121.26	127.31
52	b1	624	3PH	O21-C21-C22	4.24	120.63	111.50
48	G1	621	LUT	C21-C26-C27	4.24	118.06	112.70
49	R	621	XAT	C18-C5-C4	4.23	119.04	114.28
31	A	406	CLA	O2D-CGD-CBD	4.23	118.78	111.27
31	b	613	CLA	O2A-C1-C2	4.23	119.74	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r1	608	CLA	O2D-CGD-CBD	4.23	118.78	111.27
48	G1	621	LUT	C11-C10-C9	-4.21	121.30	127.31
35	D	411	LMG	O7-C10-C11	4.21	120.58	111.50
48	G1	620	LUT	C21-C26-C27	4.21	118.03	112.70
49	G1	622	XAT	C38-C25-C24	4.21	119.02	114.28
33	c	516	BCR	C23-C24-C25	-4.21	115.39	127.20
31	b1	609	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
49	Y	622	XAT	C18-C5-C4	4.20	119.01	114.28
35	h	102	LMG	O7-C10-C11	4.20	120.55	111.50
50	G1	623	NEX	C39-C29-C30	-4.19	117.05	122.92
49	R1	621	XAT	C15-C14-C13	-4.19	121.33	127.31
50	G1	623	NEX	C38-C25-C24	4.19	118.99	114.28
41	n1	624	LHG	O7-C7-C8	4.19	120.53	111.50
48	s	620	LUT	C18-C5-C6	-4.19	119.83	124.53
33	c	516	BCR	C33-C5-C6	-4.19	119.83	124.53
48	y	621	LUT	C21-C26-C27	4.19	117.99	112.70
48	G1	620	LUT	C7-C8-C9	-4.19	119.91	126.23
46	h1	101	RRX	C30-C25-C26	-4.18	116.72	122.61
48	n1	620	LUT	C11-C10-C9	-4.18	121.34	127.31
48	g	621	LUT	C35-C34-C33	-4.18	121.35	127.31
47	n1	609	CHL	CHD-C1D-ND	-4.18	120.61	124.45
49	n	622	XAT	C18-C5-C4	4.18	118.98	114.28
48	r1	620	LUT	C31-C30-C29	-4.17	121.35	127.31
49	n1	622	XAT	C38-C25-C24	4.17	118.97	114.28
49	Y1	622	XAT	C7-C8-C9	-4.16	119.07	125.53
31	A1	407	CLA	O2D-CGD-CBD	4.16	118.66	111.27
31	y	602	CLA	C2D-C1D-ND	4.16	113.17	110.10
33	c1	516	BCR	C33-C5-C6	-4.16	119.86	124.53
48	g	621	LUT	C15-C14-C13	-4.15	121.38	127.31
49	N	622	XAT	C7-C8-C9	-4.15	119.09	125.53
48	S	621	LUT	C11-C10-C9	-4.15	121.38	127.31
50	N	623	NEX	C16-C1-C6	-4.15	106.76	110.47
33	C1	517	BCR	C23-C22-C21	4.15	125.31	118.94
56	R1	626	ERG	C1-C2-C3	4.15	115.79	110.47
33	d	404	BCR	C19-C18-C17	4.15	125.31	118.94
31	a1	406	CLA	O2D-CGD-CBD	4.14	118.63	111.27
35	d1	411	LMG	O7-C10-C11	4.14	120.43	111.50
50	s1	623	NEX	C27-C28-C29	-4.14	119.11	125.53
33	d	404	BCR	C36-C18-C17	-4.14	117.12	122.92
48	Y1	620	LUT	C7-C8-C9	-4.14	119.98	126.23
44	D1	405	PL9	C7-C3-C2	-4.14	117.86	123.30
41	s	624	LHG	O7-C7-C8	4.13	120.41	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	t1	101	3PH	O21-C21-C22	4.13	120.41	111.50
49	G1	622	XAT	C7-C8-C9	-4.13	119.12	125.53
50	Y	623	NEX	C27-C28-C29	-4.13	119.12	125.53
37	B1	620	C7Z	C1-C6-C5	-4.13	116.79	122.61
31	B	617	CLA	C1-C2-C3	-4.13	118.90	126.04
49	Y1	622	XAT	C36-C21-C26	4.13	121.19	110.05
35	C1	523	LMG	O7-C10-C11	4.13	120.39	111.50
48	R1	620	LUT	C11-C10-C9	-4.12	121.42	127.31
48	s1	621	LUT	C31-C30-C29	-4.12	121.42	127.31
48	N1	621	LUT	C11-C10-C9	-4.12	121.43	127.31
48	R1	620	LUT	C18-C5-C6	-4.12	119.90	124.53
56	R1	626	ERG	C7-C6-C5	-4.11	115.98	123.20
31	c	512	CLA	O2D-CGD-CBD	4.11	118.57	111.27
48	y	620	LUT	C18-C5-C6	-4.11	119.91	124.53
38	c1	524	DGA	OG2-CB1-CB2	4.11	120.35	111.50
48	S	620	LUT	C22-C23-C24	-4.11	107.07	111.74
50	n	623	NEX	C2-C1-C6	4.11	113.20	109.21
48	s1	620	LUT	C22-C23-C24	-4.10	107.07	111.74
37	B1	620	C7Z	C31-C30-C29	-4.10	121.45	127.31
37	b1	620	C7Z	C7-C8-C9	-4.10	120.03	126.23
31	N	610	CLA	CAA-C2A-C3A	-4.10	101.55	112.78
31	r1	609	CLA	C1-C2-C3	-4.10	118.95	126.04
41	D	408	LHG	O7-C7-C8	4.09	120.32	111.50
49	y	622	XAT	C36-C21-C26	4.09	121.09	110.05
48	g	620	LUT	C11-C10-C9	-4.09	121.47	127.31
50	s	623	NEX	C16-C1-C6	-4.09	106.81	110.47
41	y	624	LHG	O7-C7-C8	4.09	120.31	111.50
48	N	621	LUT	C35-C34-C33	-4.08	121.49	127.31
35	C	521	LMG	O7-C10-C11	4.07	120.27	111.50
31	y	614	CLA	O2A-C1-C2	4.07	119.33	108.64
48	s1	621	LUT	C18-C5-C6	-4.07	119.96	124.53
41	D1	410	LHG	O7-C7-C8	4.06	120.26	111.50
49	Y	622	XAT	C36-C21-C26	4.06	121.02	110.05
40	c	523	DGD	O2G-C1B-C2B	4.06	120.25	111.50
49	g1	622	XAT	C38-C25-C24	4.06	118.85	114.28
31	n1	613	CLA	CAA-C2A-C3A	-4.05	101.68	112.78
48	y	621	LUT	C22-C23-C24	-4.05	107.13	111.74
47	g	601	CHL	CHD-C1D-ND	-4.05	120.73	124.45
41	C	525	LHG	O7-C7-C8	4.05	120.22	111.50
31	A1	405	CLA	CAC-C3C-C4C	-4.04	119.56	124.81
50	y1	623	NEX	C38-C25-C24	4.04	118.83	114.28
54	I1	102	4RF	O21-C22-C24	4.04	120.22	111.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	J	101	LMG	O7-C10-C11	4.04	120.21	111.50
31	B	612	CLA	CMD-C2D-C1D	4.03	131.82	124.71
31	b1	617	CLA	C2C-C1C-NC	4.03	113.75	109.97
40	C	520	DGD	O2G-C1B-C2B	4.02	120.17	111.50
48	N1	620	LUT	C22-C23-C24	-4.02	107.16	111.74
57	y1	626	PTY	O7-C8-C11	4.02	120.17	111.50
48	Y1	621	LUT	C35-C34-C33	-4.02	121.57	127.31
33	b1	618	BCR	C15-C14-C13	-4.02	121.57	127.31
47	G	608	CHL	CHD-C1D-ND	-4.02	120.76	124.45
50	G	623	NEX	C2-C1-C6	4.02	113.12	109.21
48	y1	620	LUT	C7-C8-C9	-4.02	120.16	126.23
33	c	515	BCR	C33-C5-C4	4.02	121.33	113.62
48	y1	620	LUT	C22-C23-C24	-4.01	107.18	111.74
48	y	621	LUT	C11-C10-C9	-4.01	121.59	127.31
50	G	623	NEX	C27-C28-C29	-4.00	119.32	125.53
41	c1	525	LHG	O7-C7-C8	4.00	120.13	111.50
48	g	620	LUT	C22-C23-C24	-4.00	107.19	111.74
48	S	620	LUT	C7-C8-C9	-4.00	120.19	126.23
35	h1	102	LMG	O7-C10-C11	4.00	120.12	111.50
46	H	101	RRX	C23-C24-C25	-4.00	115.98	127.20
47	n	605	CHL	CHD-C1D-ND	-3.99	120.78	124.45
31	b	617	CLA	CMD-C2D-C1D	3.99	131.75	124.71
50	G1	623	NEX	C31-C30-C29	3.99	133.01	127.31
38	b	623	DGA	OG2-CB1-CB2	3.99	120.10	111.50
31	C	502	CLA	C1-C2-C3	-3.99	119.14	126.04
48	R	620	LUT	C35-C34-C33	-3.99	121.62	127.31
48	n1	620	LUT	C21-C26-C27	3.99	117.74	112.70
50	y	623	NEX	C27-C28-C29	-3.99	119.34	125.53
31	D	402	CLA	C2D-C1D-ND	3.99	113.04	110.10
31	S1	617	CLA	C1-C2-C3	-3.98	120.31	126.75
33	c1	516	BCR	C15-C14-C13	-3.98	121.62	127.31
31	S1	611	CLA	C2C-C1C-NC	3.98	113.70	109.97
46	H1	101	RRX	C21-C20-C19	-3.98	110.80	123.22
52	s	626	3PH	O21-C21-C22	3.98	120.08	111.50
48	N	621	LUT	C15-C14-C13	-3.98	121.64	127.31
50	g	623	NEX	C2-C1-C6	3.97	113.07	109.21
33	D	404	BCR	C23-C22-C21	3.97	125.04	118.94
52	T1	101	3PH	O21-C21-C22	3.97	120.06	111.50
50	G	623	NEX	C31-C30-C29	3.97	132.97	127.31
31	S	617	CLA	C1-C2-C3	-3.97	120.34	126.75
47	G	601	CHL	CHD-C1D-ND	-3.96	120.81	124.45
48	s1	621	LUT	C21-C26-C25	3.96	118.51	111.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a1	409	PHO	CMB-C2B-C3B	3.96	132.09	124.68
33	C1	517	BCR	C37-C22-C21	-3.95	117.38	122.92
40	c1	520	DGD	O2G-C1B-C2B	3.95	120.02	111.50
48	G	620	LUT	C15-C14-C13	-3.95	121.67	127.31
46	h	101	RRX	C11-C10-C9	-3.95	121.67	127.31
52	S	626	3PH	O21-C21-C22	3.94	120.00	111.50
31	g	603	CLA	C1-C2-C3	-3.94	119.23	126.04
31	B1	614	CLA	O2D-CGD-CBD	3.94	118.27	111.27
35	B	622	LMG	O7-C10-C11	3.94	119.99	111.50
50	N	623	NEX	C27-C28-C29	-3.94	119.42	125.53
31	C	504	CLA	C1-C2-C3	-3.93	119.24	126.04
41	d1	409	LHG	O7-C7-C8	3.93	119.98	111.50
56	r1	626	ERG	C2-C1-C10	3.93	121.25	112.74
50	n	623	NEX	C38-C25-C24	3.93	118.70	114.28
35	A	413	LMG	O7-C10-C11	3.93	119.96	111.50
44	d1	405	PL9	C7-C3-C2	-3.93	118.14	123.30
48	Y	621	LUT	C7-C8-C9	-3.93	120.30	126.23
41	G1	624	LHG	O7-C7-C8	3.92	119.96	111.50
57	Y1	626	PTY	O7-C8-C11	3.92	119.96	111.50
47	Y	601	CHL	CHD-C1D-ND	-3.92	120.85	124.45
50	Y1	623	NEX	C27-C28-C29	-3.92	119.44	125.53
48	g1	620	LUT	C15-C14-C13	-3.92	121.71	127.31
48	N1	621	LUT	C7-C8-C9	-3.92	120.31	126.23
47	y1	601	CHL	CHD-C1D-ND	-3.92	120.85	124.45
31	b1	603	CLA	C1-C2-C3	-3.92	119.27	126.04
49	r	622	XAT	C18-C5-C4	3.91	118.68	114.28
38	c	524	DGA	OG2-CB1-CB2	3.91	119.93	111.50
48	r	620	LUT	C21-C26-C25	3.91	118.42	111.42
47	S	608	CHL	CHD-C1D-ND	-3.91	120.86	124.45
48	Y1	620	LUT	C35-C34-C33	-3.90	121.74	127.31
49	y1	622	XAT	C38-C25-C24	3.90	118.67	114.28
48	N	620	LUT	C7-C8-C9	-3.90	120.35	126.23
31	G	613	CLA	CMA-C3A-C4A	3.90	122.25	111.77
31	B	605	CLA	C1-C2-C3	-3.89	119.31	126.04
48	S1	620	LUT	C18-C5-C6	-3.88	120.17	124.53
31	b	615	CLA	C2C-C1C-NC	3.88	113.61	109.97
31	y1	608	CLA	C1-C2-C3	-3.88	120.47	126.75
48	G1	621	LUT	C22-C23-C24	-3.88	107.33	111.74
52	B1	624	3PH	O21-C21-C22	3.88	119.86	111.50
48	n	621	LUT	C7-C8-C9	-3.88	120.38	126.23
41	Y1	624	LHG	O7-C7-C8	3.87	119.85	111.50
47	Y1	609	CHL	CHD-C1D-ND	-3.87	120.89	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c1	516	BCR	C36-C18-C17	-3.87	117.50	122.92
50	N	623	NEX	C2-C1-C6	3.87	112.97	109.21
31	N1	602	CLA	C2D-C1D-ND	3.87	112.95	110.10
33	A	411	BCR	C33-C5-C6	-3.87	120.18	124.53
50	N1	623	NEX	C27-C28-C29	-3.86	119.54	125.53
50	Y	623	NEX	C39-C29-C30	-3.86	117.51	122.92
35	a1	413	LMG	O7-C10-C11	3.86	119.82	111.50
33	d1	404	BCR	C1-C6-C5	-3.86	117.18	122.61
47	N1	605	CHL	CHD-C1D-ND	-3.85	120.91	124.45
48	R1	620	LUT	C21-C26-C25	3.85	118.32	111.42
47	Y	605	CHL	CHD-C1D-ND	-3.85	120.91	124.45
48	y1	620	LUT	C18-C5-C6	-3.85	120.20	124.53
35	j	101	LMG	O7-C10-C11	3.85	119.80	111.50
47	s1	607	CHL	CHD-C1D-ND	-3.85	120.92	124.45
49	y	622	XAT	C38-C25-C24	3.85	118.61	114.28
35	C1	521	LMG	O7-C10-C11	3.85	119.79	111.50
38	B	625	DGA	OG2-CB1-CB2	3.85	119.79	111.50
47	g	606	CHL	C2C-C3C-C4C	3.84	109.23	106.49
46	H	101	RRX	C33-C5-C4	3.84	121.00	113.62
47	s1	608	CHL	CHD-C1D-ND	-3.84	120.92	124.45
50	Y	623	NEX	C31-C30-C29	3.84	132.79	127.31
38	C	524	DGA	OG2-CB1-CB2	3.84	119.78	111.50
48	N1	621	LUT	C22-C23-C24	-3.84	107.37	111.74
47	g1	609	CHL	CHD-C1D-ND	-3.83	120.93	124.45
31	n	613	CLA	CMA-C3A-C4A	3.83	122.08	111.77
50	y	623	NEX	C39-C29-C30	-3.83	117.55	122.92
50	y1	623	NEX	C31-C30-C29	3.83	132.78	127.31
48	g1	621	LUT	C22-C23-C24	-3.83	107.38	111.74
33	B	618	BCR	C23-C24-C25	-3.83	116.45	127.20
31	c1	513	CLA	C1-C2-C3	-3.83	119.42	126.04
41	Y	624	LHG	O7-C7-C8	3.83	119.75	111.50
48	Y	621	LUT	C11-C10-C9	-3.82	121.85	127.31
54	i1	101	4RF	O21-C22-C24	3.82	119.74	111.50
33	d	404	BCR	C4-C5-C6	-3.82	117.19	122.73
50	Y	623	NEX	C17-C1-C6	-3.82	107.06	110.47
48	S1	621	LUT	C18-C5-C6	-3.82	120.24	124.53
38	J1	101	DGA	OG2-CB1-CB2	3.82	119.72	111.50
33	B	618	BCR	C15-C14-C13	-3.81	121.87	127.31
48	Y	620	LUT	C31-C30-C29	-3.81	121.87	127.31
31	c	511	CLA	C1-C2-C3	-3.81	119.45	126.04
48	y1	621	LUT	C7-C8-C9	-3.81	120.48	126.23
48	N1	620	LUT	C35-C34-C33	-3.81	121.87	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	g1	623	NEX	C27-C28-C29	-3.81	119.62	125.53
48	G	621	LUT	C15-C14-C13	-3.81	121.88	127.31
33	D	404	BCR	C37-C22-C21	-3.80	117.59	122.92
33	B1	619	BCR	C33-C5-C4	3.80	120.92	113.62
47	S1	608	CHL	C4A-NA-C1A	3.80	108.42	106.71
31	B	615	CLA	CBA-CAA-C2A	3.80	125.08	113.86
33	D	404	BCR	C36-C18-C17	-3.80	117.60	122.92
31	Y1	608	CLA	C1-C2-C3	-3.80	120.61	126.75
31	s	609	CLA	CMA-C3A-C4A	3.80	121.97	111.77
50	n1	623	NEX	C38-C25-C24	3.79	118.55	114.28
46	H1	101	RRX	C4-C5-C6	-3.79	117.23	122.73
50	n1	623	NEX	C27-C28-C29	-3.79	119.65	125.53
50	n1	623	NEX	C39-C29-C30	-3.79	117.61	122.92
46	H1	101	RRX	C1-C6-C5	-3.79	117.28	122.61
50	s1	623	NEX	C19-C9-C10	-3.79	117.62	122.92
42	c	627	LMK	O3-C4-C3	-3.78	110.01	122.98
50	G	623	NEX	C39-C29-C30	-3.77	117.64	122.92
40	c	518	DGD	O2G-C1B-C2B	3.77	119.64	111.50
34	B	621	SQD	O7-S-C6	-3.77	102.45	106.94
35	d	411	LMG	O7-C10-C11	3.77	119.63	111.50
34	m1	101	SQD	O7-S-C6	-3.77	102.46	106.94
56	R1	626	ERG	C2-C1-C10	3.77	120.90	112.74
41	d1	408	LHG	O7-C7-C8	3.77	119.62	111.50
31	s	617	CLA	C1-C2-C3	-3.77	120.66	126.75
41	c	625	LHG	O7-C7-C8	3.77	119.62	111.50
31	S	604	CLA	C1-C2-C3	-3.77	119.53	126.04
48	y	621	LUT	C35-C34-C33	-3.76	121.94	127.31
37	B1	620	C7Z	C27-C28-C29	-3.76	120.55	126.23
38	j1	101	DGA	OG2-CB1-CB2	3.76	119.61	111.50
40	c1	519	DGD	O2G-C1B-C2B	3.76	119.60	111.50
47	G1	608	CHL	CHD-C1D-ND	-3.76	121.00	124.45
38	C1	524	DGA	OG2-CB1-CB2	3.76	119.60	111.50
47	N	609	CHL	CHD-C1D-ND	-3.76	121.00	124.45
41	s1	624	LHG	O7-C7-C8	3.76	119.59	111.50
54	k1	101	4RF	O21-C22-C24	3.75	119.59	111.50
31	b1	602	CLA	C2C-C1C-NC	3.75	113.49	109.97
50	R1	622	NEX	C27-C28-C29	-3.75	119.71	125.53
31	b	606	CLA	C2C-C1C-NC	3.75	113.49	109.97
31	Y1	610	CLA	C2D-C1D-ND	3.75	112.87	110.10
46	h	101	RRX	C1-C6-C5	-3.75	117.33	122.61
31	B1	605	CLA	C1-C2-C3	-3.75	119.56	126.04
31	c	511	CLA	CMA-C3A-C4A	3.75	121.85	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	410	CLA	C1-C2-C3	-3.75	119.56	126.04
49	g	622	XAT	O4-C5-C4	-3.75	110.57	113.38
48	Y1	620	LUT	C21-C26-C27	3.75	117.44	112.70
31	b1	603	CLA	C1-O2A-CGA	3.75	126.27	116.44
48	G1	620	LUT	C31-C30-C29	-3.74	121.97	127.31
49	R	621	XAT	C38-C25-C26	-3.74	115.99	122.26
48	g1	621	LUT	C7-C8-C9	-3.74	120.58	126.23
31	R1	609	CLA	C1-C2-C3	-3.74	119.57	126.04
34	a	412	SQD	O7-S-C6	-3.74	102.49	106.94
47	S	601	CHL	CHD-C1D-ND	-3.74	121.02	124.45
40	c	519	DGD	O2G-C1B-C2B	3.74	119.55	111.50
48	g1	621	LUT	C11-C10-C9	-3.73	121.98	127.31
47	n1	605	CHL	CHD-C1D-ND	-3.73	121.02	124.45
31	s1	611	CLA	OBD-CAD-C3D	-3.73	119.55	128.52
31	G1	602	CLA	C2D-C1D-ND	3.73	112.85	110.10
34	B1	626	SQD	O7-S-C6	-3.73	102.51	106.94
32	A	409	PHO	CMB-C2B-C3B	3.73	131.65	124.68
50	G1	623	NEX	C2-C1-C6	3.73	112.83	109.21
48	S	620	LUT	C15-C14-C13	-3.73	121.99	127.31
48	n	621	LUT	C11-C10-C9	-3.72	122.00	127.31
47	S1	606	CHL	CHD-C1D-ND	-3.72	121.03	124.45
48	s1	621	LUT	C11-C10-C9	-3.72	122.00	127.31
31	s1	605	CLA	C2C-C1C-NC	3.72	113.45	109.97
34	b1	621	SQD	O7-S-C6	-3.71	102.52	106.94
35	H1	102	LMG	O7-C10-C11	3.71	119.51	111.50
50	s	623	NEX	C17-C1-C6	-3.71	107.15	110.47
31	b	605	CLA	C2C-C1C-NC	3.71	113.45	109.97
50	S	622	NEX	C27-C28-C29	-3.71	119.77	125.53
31	N1	610	CLA	CHD-C1D-ND	-3.71	121.05	124.45
49	r	622	XAT	C26-C27-C28	-3.71	118.15	125.99
31	n	611	CLA	C2D-C1D-ND	3.71	112.83	110.10
47	y1	609	CHL	CHD-C1D-ND	-3.70	121.05	124.45
31	B	615	CLA	CAA-C2A-C3A	-3.70	102.64	112.78
31	g1	603	CLA	C1-C2-C3	-3.70	119.64	126.04
47	N	605	CHL	CHD-C1D-ND	-3.70	121.05	124.45
31	n	610	CLA	C2D-C1D-ND	3.70	112.83	110.10
47	Y1	601	CHL	CHD-C1D-ND	-3.70	121.06	124.45
40	C1	520	DGD	O2G-C1B-C2B	3.70	119.47	111.50
48	G	620	LUT	C35-C34-C33	-3.70	122.03	127.31
48	s	621	LUT	C31-C30-C29	-3.70	122.04	127.31
47	g1	606	CHL	CHD-C1D-ND	-3.69	121.06	124.45
47	s	606	CHL	CHD-C1D-ND	-3.69	121.06	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	615	CLA	CAA-C2A-C3A	-3.69	102.67	112.78
50	g1	623	NEX	C31-C30-C29	3.69	132.58	127.31
31	S1	613	CLA	C1-C2-C3	-3.69	119.67	126.04
48	Y	620	LUT	C15-C35-C34	-3.69	115.92	123.47
33	C	515	BCR	C33-C5-C6	-3.69	120.39	124.53
31	A	406	CLA	C1-C2-C3	-3.68	119.67	126.04
37	b1	620	C7Z	C35-C34-C33	-3.68	122.05	127.31
48	g1	620	LUT	C22-C23-C24	-3.68	107.55	111.74
31	g	602	CLA	CHD-C1D-ND	-3.68	121.07	124.45
47	s	601	CHL	CHD-C1D-ND	-3.68	121.07	124.45
34	a1	412	SQD	O7-S-C6	-3.68	102.57	106.94
33	C1	515	BCR	C33-C5-C6	-3.68	120.40	124.53
47	g1	601	CHL	CHD-C1D-ND	-3.68	121.08	124.45
47	y1	607	CHL	C4A-NA-C1A	3.68	108.36	106.71
46	H	101	RRX	C1-C6-C5	-3.67	117.44	122.61
31	s1	613	CLA	C2C-C1C-NC	3.67	113.41	109.97
31	Y1	610	CLA	C1-C2-C3	-3.67	119.70	126.04
31	s1	613	CLA	C1-C2-C3	-3.67	119.70	126.04
31	r	603	CLA	O2A-C1-C2	3.67	118.27	108.64
31	Y1	602	CLA	CHD-C1D-ND	-3.67	121.08	124.45
31	y1	614	CLA	CHD-C1D-ND	-3.66	121.09	124.45
47	S1	608	CHL	CHD-C1D-ND	-3.66	121.09	124.45
31	C1	508	CLA	C2D-C1D-ND	3.66	112.80	110.10
48	s1	620	LUT	C18-C5-C6	-3.66	120.41	124.53
31	G1	613	CLA	C1-C2-C3	-3.66	119.71	126.04
48	G1	621	LUT	C15-C14-C13	-3.66	122.08	127.31
50	Y	623	NEX	C19-C9-C10	-3.66	117.80	122.92
41	l	101	LHG	O7-C7-C8	3.66	119.39	111.50
37	B	620	C7Z	C31-C30-C29	-3.66	122.09	127.31
31	b1	610	CLA	C2C-C1C-NC	3.66	113.40	109.97
47	N	607	CHL	C4A-NA-C1A	3.66	108.35	106.71
34	M1	101	SQD	O7-S-C6	-3.66	102.59	106.94
47	g	608	CHL	CHD-C1D-ND	-3.66	121.09	124.45
31	s	605	CLA	C1-C2-C3	-3.65	120.84	126.75
40	c1	518	DGD	O2G-C1B-C2B	3.65	119.38	111.50
31	C1	509	CLA	O2A-C1-C2	3.65	118.23	108.64
42	c1	527	LMK	O3-C4-C3	-3.65	110.45	122.98
47	n	601	CHL	CHD-C1D-ND	-3.65	121.10	124.45
41	d	409	LHG	O7-C7-C8	3.65	119.37	111.50
31	c	503	CLA	C1-C2-C3	-3.65	119.73	126.04
33	B1	618	BCR	C33-C5-C4	3.65	120.62	113.62
47	g	605	CHL	CHD-C1D-ND	-3.65	121.10	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	609	CLA	CMB-C2B-C3B	3.64	131.50	124.68
41	y1	624	LHG	O7-C7-C8	3.64	119.36	111.50
48	S	621	LUT	C7-C8-C9	-3.64	120.73	126.23
31	b1	605	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
47	n	608	CHL	C4A-NA-C1A	3.64	108.34	106.71
33	c1	517	BCR	C15-C14-C13	-3.64	122.12	127.31
56	r1	626	ERG	C7-C6-C5	-3.64	116.81	123.20
31	g	610	CLA	C1-C2-C3	-3.64	119.75	126.04
48	y	620	LUT	C22-C23-C24	-3.64	107.60	111.74
35	H	102	LMG	O7-C10-C11	3.64	119.34	111.50
46	h1	101	RRX	C21-C20-C19	-3.63	111.88	123.22
56	R1	626	ERG	C18-C13-C12	-3.63	104.85	110.59
34	b1	626	SQD	O7-S-C6	-3.63	102.62	106.94
50	y	623	NEX	C38-C25-C24	3.63	118.37	114.28
31	B1	612	CLA	C1-C2-C3	-3.63	119.76	126.04
31	Y1	603	CLA	C2C-C1C-NC	3.63	113.37	109.97
31	N	610	CLA	CMA-C3A-C4A	3.63	121.53	111.77
34	C	526	SQD	O7-S-C6	-3.63	102.62	106.94
50	S	622	NEX	C2-C1-C6	3.63	112.74	109.21
50	y1	623	NEX	C27-C28-C29	-3.63	119.90	125.53
34	A	412	SQD	O7-S-C6	-3.63	102.63	106.94
40	C1	518	DGD	O2G-C1B-C2B	3.63	119.32	111.50
31	C	504	CLA	CHD-C1D-ND	-3.63	121.12	124.45
48	N1	621	LUT	C15-C14-C13	-3.63	122.13	127.31
46	h1	101	RRX	C37-C22-C23	3.62	123.79	118.08
35	c1	523	LMG	O7-C10-C11	3.62	119.31	111.50
47	G	609	CHL	CHD-C1D-ND	-3.62	121.12	124.45
47	S	606	CHL	CHD-C1D-ND	-3.62	121.13	124.45
50	s1	623	NEX	C39-C29-C30	-3.62	117.85	122.92
31	C1	510	CLA	C2C-C1C-NC	3.62	113.36	109.97
31	N1	604	CLA	C1-C2-C3	-3.62	119.79	126.04
34	C1	526	SQD	O7-S-C6	-3.62	102.64	106.94
48	G1	621	LUT	C31-C30-C29	-3.61	122.15	127.31
33	c	515	BCR	C23-C24-C25	-3.61	117.06	127.20
31	A1	407	CLA	CHD-C1D-ND	-3.61	121.14	124.45
31	n1	602	CLA	C1-C2-C3	-3.61	119.80	126.04
48	s	621	LUT	C22-C23-C24	-3.60	107.64	111.74
48	s1	620	LUT	C15-C14-C13	-3.60	122.17	127.31
31	B1	609	CLA	C2C-C1C-NC	3.60	113.35	109.97
33	b	619	BCR	C36-C18-C17	-3.60	117.88	122.92
33	B1	618	BCR	C1-C6-C5	-3.60	117.55	122.61
33	b1	619	BCR	C33-C5-C4	3.60	120.53	113.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	N1	608	CHL	CHD-C1D-ND	-3.60	121.15	124.45
35	D1	411	LMG	O7-C10-C11	3.60	119.25	111.50
50	G	623	NEX	C17-C1-C6	-3.60	107.25	110.47
48	S1	620	LUT	C35-C15-C14	-3.60	116.11	123.47
48	y1	620	LUT	C35-C34-C33	-3.60	122.18	127.31
48	N	620	LUT	C21-C26-C27	3.59	117.25	112.70
31	b1	609	CLA	C1-C2-C3	-3.59	119.83	126.04
50	s1	623	NEX	C31-C30-C29	3.59	132.44	127.31
31	s	613	CLA	C1-C2-C3	-3.59	119.83	126.04
47	G	607	CHL	CHB-C4A-NA	3.59	129.48	124.51
31	c	508	CLA	C1-C2-C3	-3.59	119.83	126.04
31	B1	611	CLA	C2C-C1C-NC	3.59	113.33	109.97
31	a	405	CLA	CHD-C1D-ND	-3.59	121.16	124.45
31	r1	608	CLA	C2C-C1C-NC	3.59	113.33	109.97
37	b	620	C7Z	C27-C28-C29	-3.59	120.82	126.23
31	S1	604	CLA	C1-C2-C3	-3.59	119.84	126.04
38	b1	625	DGA	OG2-CB1-CB2	3.59	119.23	111.50
31	B	603	CLA	C1-C2-C3	-3.58	119.84	126.04
50	S	622	NEX	C17-C1-C6	-3.58	107.27	110.47
49	r1	621	XAT	C7-C8-C9	-3.58	119.97	125.53
31	c1	501	CLA	C1-C2-C3	-3.58	119.85	126.04
47	s	608	CHL	CHD-C1D-ND	-3.58	121.17	124.45
37	B	620	C7Z	C1-C6-C5	-3.58	117.57	122.61
48	R1	620	LUT	C7-C8-C9	-3.57	120.83	126.23
31	A	407	CLA	C2C-C1C-NC	3.57	113.32	109.97
47	s1	606	CHL	CHD-C1D-ND	-3.57	121.17	124.45
49	y	622	XAT	O4-C5-C4	-3.57	110.70	113.38
31	a	405	CLA	C2D-C1D-ND	3.57	112.74	110.10
31	C	511	CLA	CHD-C1D-ND	-3.57	121.17	124.45
31	n	610	CLA	CAA-C2A-C3A	-3.57	103.00	112.78
47	r	606	CHL	CHD-C1D-ND	-3.57	121.17	124.45
33	c1	516	BCR	C19-C18-C17	3.57	124.42	118.94
47	N1	601	CHL	CHD-C1D-ND	-3.57	121.18	124.45
33	A1	411	BCR	C33-C5-C6	-3.57	120.52	124.53
48	N	621	LUT	C22-C23-C24	-3.56	107.69	111.74
31	s	604	CLA	CHD-C1D-ND	-3.56	121.18	124.45
50	n	623	NEX	C39-C29-C30	-3.56	117.93	122.92
31	b1	609	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
31	G	612	CLA	C2C-C1C-NC	3.56	113.31	109.97
48	g	621	LUT	C18-C5-C6	-3.56	120.53	124.53
31	G1	610	CLA	CHD-C1D-ND	-3.56	121.18	124.45
47	N1	606	CHL	CHD-C1D-ND	-3.56	121.18	124.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	H1	101	RRX	C33-C5-C6	-3.56	120.53	124.53
46	H	101	RRX	C24-C23-C22	3.56	131.61	126.23
31	Y1	613	CLA	CHD-C1D-ND	-3.56	121.19	124.45
31	C	509	CLA	C1-C2-C3	-3.55	119.90	126.04
31	A	406	CLA	C2C-C1C-NC	3.55	113.30	109.97
31	C1	509	CLA	C2C-C1C-NC	3.55	113.30	109.97
47	G1	601	CHL	C2C-C3C-C4C	3.55	109.02	106.49
31	R	610	CLA	CMA-C3A-C4A	3.55	121.32	111.77
33	c	515	BCR	C4-C5-C6	-3.55	117.57	122.73
40	C1	519	DGD	O2G-C1B-C2B	3.55	119.16	111.50
48	N	620	LUT	C11-C10-C9	-3.55	122.25	127.31
49	G	622	XAT	C7-C8-C9	-3.55	120.03	125.53
48	S	621	LUT	C22-C23-C24	-3.55	107.70	111.74
49	g	622	XAT	C6-C7-C8	-3.55	118.50	125.99
31	S1	613	CLA	C2C-C1C-NC	3.54	113.29	109.97
50	Y	623	NEX	C11-C10-C9	3.54	132.37	127.31
31	G	610	CLA	C2D-C1D-ND	3.54	112.72	110.10
31	B	606	CLA	CHD-C1D-ND	-3.54	121.20	124.45
34	A1	412	SQD	O7-S-C6	-3.54	102.73	106.94
46	h1	101	RRX	C33-C5-C4	3.54	120.42	113.62
31	R1	610	CLA	C1-C2-C3	-3.54	119.92	126.04
31	b	604	CLA	C2C-C1C-NC	3.54	113.29	109.97
47	Y	605	CHL	C2C-C3C-C4C	3.54	109.01	106.49
47	G	605	CHL	CHD-C1D-ND	-3.54	121.20	124.45
31	B	605	CLA	C2C-C1C-NC	3.54	113.28	109.97
33	b1	618	BCR	C33-C5-C6	-3.53	120.56	124.53
34	B1	621	SQD	O7-S-C6	-3.53	102.74	106.94
48	y	621	LUT	C15-C14-C13	-3.53	122.27	127.31
31	s	614	CLA	C1-C2-C3	-3.53	119.94	126.04
31	A1	405	CLA	C1-C2-C3	-3.53	119.94	126.04
44	D	405	PL9	C7-C3-C2	-3.53	118.66	123.30
31	s	613	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
31	y1	611	CLA	C1-C2-C3	-3.53	119.94	126.04
31	G1	611	CLA	C2C-C1C-NC	3.53	113.28	109.97
47	G1	606	CHL	C2C-C3C-C4C	3.53	109.00	106.49
48	R	620	LUT	C7-C8-C9	-3.53	120.91	126.23
47	n	606	CHL	CHD-C1D-ND	-3.53	121.21	124.45
47	y1	606	CHL	CHD-C1D-ND	-3.53	121.21	124.45
31	s	617	CLA	CHD-C1D-ND	-3.52	121.22	124.45
50	g	623	NEX	C16-C1-C6	-3.52	107.32	110.47
31	d	403	CLA	C2C-C1C-NC	3.52	113.27	109.97
31	g	603	CLA	C2C-C1C-NC	3.52	113.27	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A1	405	CLA	CHD-C1D-ND	-3.52	121.22	124.45
31	s1	604	CLA	C2C-C1C-NC	3.52	113.27	109.97
47	g	609	CHL	CHD-C1D-ND	-3.52	121.22	124.45
47	G1	601	CHL	CHD-C1D-ND	-3.52	121.22	124.45
31	g	610	CLA	CHD-C1D-ND	-3.52	121.22	124.45
48	S	621	LUT	C18-C5-C6	-3.52	120.57	124.53
49	R1	621	XAT	C7-C8-C9	-3.52	120.07	125.53
31	c	507	CLA	C2C-C1C-NC	3.52	113.27	109.97
47	n	609	CHL	CMA-C3A-C4A	3.52	121.23	111.77
48	S1	621	LUT	C35-C15-C14	-3.52	116.26	123.47
46	h1	101	RRX	C4-C5-C6	-3.52	117.62	122.73
31	S	611	CLA	C2C-C1C-NC	3.52	113.27	109.97
47	S	607	CHL	CHD-C1D-ND	-3.52	121.22	124.45
34	c	626	SQD	O7-S-C6	-3.52	102.76	106.94
33	b1	618	BCR	C27-C26-C25	-3.52	117.63	122.73
50	N1	623	NEX	C31-C30-C29	3.52	132.33	127.31
31	s	613	CLA	C2C-C1C-NC	3.52	113.27	109.97
47	r1	606	CHL	CHD-C1D-ND	-3.51	121.22	124.45
31	g	603	CLA	C2D-C1D-ND	3.51	112.69	110.10
31	b	617	CLA	C1-C2-C3	-3.51	119.97	126.04
33	c1	517	BCR	C37-C22-C21	-3.51	118.00	122.92
47	Y	605	CHL	C3C-C4C-NC	-3.51	106.63	110.57
47	y1	605	CHL	CHD-C1D-ND	-3.51	121.23	124.45
48	Y1	620	LUT	C22-C23-C24	-3.51	107.75	111.74
46	h	101	RRX	C33-C5-C4	3.51	120.36	113.62
31	n	610	CLA	CHD-C1D-ND	-3.51	121.23	124.45
31	D1	402	CLA	C2D-C1D-ND	3.51	112.69	110.10
31	C	508	CLA	C1-C2-C3	-3.51	119.98	126.04
42	C	527	LMK	O3-C4-C3	-3.51	110.95	122.98
38	B1	625	DGA	OG2-CB1-CB2	3.51	119.06	111.50
31	n	602	CLA	CHD-C1D-ND	-3.50	121.23	124.45
47	r	607	CHL	CHD-C1D-ND	-3.50	121.23	124.45
31	G	603	CLA	C2C-C1C-NC	3.50	113.25	109.97
47	g	608	CHL	C4A-NA-C1A	3.50	108.28	106.71
31	Y	613	CLA	C1-C2-C3	-3.50	119.98	126.04
31	A	410	CLA	C2C-C1C-NC	3.50	113.25	109.97
47	N	601	CHL	CHD-C1D-ND	-3.50	121.24	124.45
47	G1	609	CHL	CHD-C1D-ND	-3.50	121.24	124.45
47	S1	607	CHL	CHD-C1D-ND	-3.50	121.24	124.45
40	C	518	DGD	O2G-C1B-C2B	3.50	119.04	111.50
31	C1	512	CLA	C1-C2-C3	-3.50	119.99	126.04
31	r1	603	CLA	C2C-C1C-NC	3.50	113.25	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	h1	101	RRX	C16-C17-C18	-3.50	122.32	127.31
48	N	620	LUT	C31-C30-C29	-3.50	122.32	127.31
34	c1	526	SQD	O7-S-C6	-3.49	102.79	106.94
47	N	607	CHL	CHB-C4A-NA	3.49	129.34	124.51
31	r	603	CLA	C2C-C1C-NC	3.49	113.24	109.97
31	y	613	CLA	C2C-C1C-NC	3.49	113.24	109.97
31	G	604	CLA	CMA-C3A-C4A	3.49	121.16	111.77
41	D	410	LHG	O7-C7-C8	3.49	119.03	111.50
49	r1	621	XAT	C26-C27-C28	-3.49	118.61	125.99
47	y1	605	CHL	C2C-C3C-C4C	3.49	108.98	106.49
49	y	622	XAT	C7-C8-C9	-3.49	120.11	125.53
31	B1	616	CLA	C2C-C1C-NC	3.49	113.24	109.97
33	c	517	BCR	C15-C14-C13	-3.49	122.33	127.31
48	G1	620	LUT	C11-C10-C9	-3.49	122.33	127.31
48	y1	620	LUT	C15-C14-C13	-3.49	122.33	127.31
50	S	622	NEX	C39-C29-C30	-3.48	118.04	122.92
34	b	621	SQD	O7-S-C6	-3.48	102.80	106.94
47	G	606	CHL	C2C-C3C-C4C	3.48	108.97	106.49
33	b1	618	BCR	C33-C5-C4	3.48	120.31	113.62
49	r	622	XAT	C19-C9-C10	-3.48	118.05	122.92
48	N	620	LUT	C18-C5-C6	-3.48	120.62	124.53
31	c	505	CLA	C1-C2-C3	-3.48	120.02	126.04
33	B	619	BCR	C33-C5-C6	-3.48	120.62	124.53
33	c1	517	BCR	C33-C5-C6	-3.48	120.62	124.53
31	C1	510	CLA	CHD-C1D-ND	-3.48	121.25	124.45
31	c1	502	CLA	C2C-C1C-NC	3.48	113.23	109.97
31	b1	603	CLA	C2C-C1C-NC	3.48	113.23	109.97
31	S	613	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
50	y1	623	NEX	C39-C29-C30	-3.47	118.06	122.92
31	c1	511	CLA	C1-C2-C3	-3.47	120.05	126.04
47	N1	601	CHL	C3C-C4C-NC	-3.47	106.68	110.57
31	b	609	CLA	C1-C2-C3	-3.46	120.05	126.04
31	a1	406	CLA	CHD-C1D-ND	-3.46	121.27	124.45
47	S1	601	CHL	CHD-C1D-ND	-3.46	121.27	124.45
31	b1	613	CLA	C2C-C1C-NC	3.46	113.22	109.97
33	a	411	BCR	C23-C24-C25	-3.46	117.48	127.20
31	G1	610	CLA	C1-C2-C3	-3.46	120.06	126.04
31	B1	615	CLA	C2C-C1C-NC	3.46	113.22	109.97
47	n1	601	CHL	CHD-C1D-ND	-3.46	121.27	124.45
31	B	609	CLA	C2C-C1C-NC	3.46	113.21	109.97
33	B	619	BCR	C33-C5-C4	3.46	120.26	113.62
31	B	611	CLA	C2D-C1D-ND	3.46	112.65	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	613	CLA	C2C-C1C-NC	3.46	113.21	109.97
49	r1	621	XAT	C15-C14-C13	-3.46	122.37	127.31
31	G	610	CLA	CHD-C1D-ND	-3.46	121.28	124.45
31	c	510	CLA	C1-C2-C3	-3.46	120.06	126.04
48	Y	621	LUT	C15-C14-C13	-3.46	122.37	127.31
31	R	603	CLA	CMA-C3A-C4A	3.46	121.07	111.77
31	b1	604	CLA	CHD-C1D-ND	-3.46	121.28	124.45
31	B1	606	CLA	C2C-C1C-NC	3.45	113.21	109.97
31	c	504	CLA	C1-C2-C3	-3.45	120.07	126.04
47	N1	605	CHL	C3C-C4C-NC	-3.45	106.70	110.57
31	s1	610	CLA	C2C-C1C-NC	3.45	113.21	109.97
47	N	606	CHL	CHD-C1D-ND	-3.45	121.28	124.45
31	S1	609	CLA	CHD-C1D-ND	-3.45	121.28	124.45
31	y1	608	CLA	CHD-C1D-ND	-3.45	121.28	124.45
47	Y	609	CHL	CHD-C1D-ND	-3.45	121.28	124.45
31	Y1	613	CLA	C2C-C1C-NC	3.45	113.20	109.97
31	C1	509	CLA	CHD-C1D-ND	-3.45	121.28	124.45
31	A1	406	CLA	CMB-C2B-C3B	3.45	131.13	124.68
31	s1	602	CLA	CHD-C1D-ND	-3.45	121.28	124.45
31	A1	407	CLA	C1-C2-C3	-3.45	121.17	126.75
48	g1	620	LUT	C11-C10-C9	-3.45	122.39	127.31
37	b1	620	C7Z	C18-C5-C4	3.45	120.74	114.36
31	A	406	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
31	s	614	CLA	C2C-C1C-NC	3.44	113.20	109.97
31	C1	510	CLA	C1-C2-C3	-3.44	120.09	126.04
31	b	616	CLA	C2C-C1C-NC	3.44	113.20	109.97
31	c1	504	CLA	C2C-C1C-NC	3.44	113.20	109.97
47	G1	605	CHL	CHD-C1D-ND	-3.44	121.29	124.45
31	y	604	CLA	C2C-C1C-NC	3.44	113.19	109.97
31	r1	602	CLA	C1-C2-C3	-3.44	120.09	126.04
47	G1	601	CHL	C3C-C4C-NC	-3.44	106.71	110.57
33	D1	404	BCR	C36-C18-C17	-3.44	118.11	122.92
49	g	622	XAT	C38-C25-C26	-3.44	116.50	122.26
31	n1	610	CLA	CAA-C2A-C3A	-3.44	103.36	112.78
31	G	613	CLA	CAC-C3C-C4C	3.44	129.27	124.81
48	S	620	LUT	C18-C5-C6	-3.44	120.67	124.53
31	c1	508	CLA	C2D-C1D-ND	3.44	112.64	110.10
31	s1	617	CLA	CMA-C3A-C4A	3.44	121.01	111.77
33	d1	404	BCR	C4-C5-C6	-3.44	117.74	122.73
31	C	506	CLA	CHD-C1D-ND	-3.43	121.30	124.45
47	n	609	CHL	CHD-C1D-ND	-3.43	121.30	124.45
31	a1	407	CLA	C2C-C1C-NC	3.43	113.19	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	612	CLA	C2C-C1C-NC	3.43	113.19	109.97
31	g	602	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
48	r	620	LUT	C11-C10-C9	-3.43	122.41	127.31
31	B1	605	CLA	C2D-C1D-ND	3.43	112.63	110.10
31	s	610	CLA	C1-O2A-CGA	3.43	125.44	116.44
37	b1	620	C7Z	C18-C5-C6	-3.43	120.68	124.53
50	N1	623	NEX	C5-C4-C3	3.43	115.81	111.75
50	R1	622	NEX	C1-C2-C3	3.43	121.39	113.64
31	g	613	CLA	CMA-C3A-C4A	3.43	120.99	111.77
31	b	609	CLA	C2C-C1C-NC	3.43	113.18	109.97
31	c1	509	CLA	O2A-C1-C2	3.43	117.64	108.64
46	h	101	RRX	C4-C5-C6	-3.43	117.75	122.73
31	s1	617	CLA	CHD-C1D-ND	-3.43	121.31	124.45
47	n1	601	CHL	C2C-C3C-C4C	3.43	108.93	106.49
31	S	617	CLA	CMA-C3A-C4A	3.43	120.98	111.77
31	n	604	CLA	C1-C2-C3	-3.42	120.12	126.04
49	R1	621	XAT	O4-C5-C4	-3.42	110.81	113.38
33	c1	517	BCR	C35-C13-C14	-3.42	118.13	122.92
31	d1	403	CLA	C1-C2-C3	-3.42	120.12	126.04
31	b	612	CLA	C2D-C1D-ND	3.42	112.63	110.10
47	N1	605	CHL	C2C-C3C-C4C	3.42	108.93	106.49
31	S	605	CLA	C1-C2-C3	-3.42	121.22	126.75
31	N1	613	CLA	CMA-C3A-C4A	3.42	120.96	111.77
46	H	101	RRX	C38-C26-C25	-3.42	120.69	124.53
49	r	622	XAT	C38-C25-C26	-3.42	116.53	122.26
31	c1	505	CLA	C1-C2-C3	-3.42	120.13	126.04
31	y	614	CLA	C2C-C1C-NC	3.42	113.17	109.97
31	g1	612	CLA	C2C-C1C-NC	3.41	113.17	109.97
47	R1	607	CHL	CHD-C1D-ND	-3.41	121.32	124.45
31	c	504	CLA	CMA-C3A-C4A	3.41	120.95	111.77
31	b1	609	CLA	C2C-C1C-NC	3.41	113.17	109.97
31	c	503	CLA	CHD-C1D-ND	-3.41	121.32	124.45
31	d	403	CLA	C1-C2-C3	-3.41	120.14	126.04
50	G1	623	NEX	C27-C28-C29	-3.41	120.24	125.53
31	a	407	CLA	C2C-C1C-NC	3.41	113.17	109.97
31	B	602	CLA	CMA-C3A-C4A	3.41	120.94	111.77
47	Y1	605	CHL	CHD-C1D-ND	-3.41	121.32	124.45
48	n	621	LUT	C31-C30-C29	-3.41	122.45	127.31
45	F	101	HEM	C4B-CHC-C1C	3.41	127.06	122.56
33	C1	516	BCR	C37-C22-C21	-3.41	118.15	122.92
48	r1	620	LUT	C18-C5-C6	-3.41	120.70	124.53
50	g1	623	NEX	C39-C29-C30	-3.41	118.15	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	N	608	CHL	CHD-C1D-ND	-3.40	121.33	124.45
31	S1	603	CLA	C2C-C1C-NC	3.40	113.16	109.97
31	S	612	CLA	C2C-C1C-NC	3.40	113.16	109.97
47	g1	601	CHL	CMA-C3A-C4A	3.40	120.91	111.77
31	C1	509	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
54	K1	101	4RF	O21-C22-C24	3.40	118.82	111.50
31	b1	615	CLA	C2C-C1C-NC	3.39	113.15	109.97
31	c1	503	CLA	CHD-C1D-ND	-3.39	121.33	124.45
48	G1	620	LUT	C22-C23-C24	-3.39	107.88	111.74
47	S	607	CHL	CMA-C3A-C4A	3.39	120.89	111.77
31	B	615	CLA	CMB-C2B-C3B	3.39	131.02	124.68
48	N	621	LUT	C18-C5-C6	-3.39	120.72	124.53
31	n	612	CLA	CHD-C1D-ND	-3.39	121.34	124.45
31	R	610	CLA	CHD-C1D-ND	-3.39	121.34	124.45
31	G1	613	CLA	CMA-C3A-C4A	3.39	120.88	111.77
49	n	622	XAT	C38-C25-C26	-3.39	116.58	122.26
45	f	101	HEM	C3B-C2B-C1B	3.39	109.00	106.49
31	C1	506	CLA	C2D-C1D-ND	3.39	112.60	110.10
31	s1	614	CLA	C2C-C1C-NC	3.39	113.15	109.97
46	H	101	RRX	C33-C5-C6	-3.39	120.72	124.53
49	R	621	XAT	C19-C9-C10	-3.39	118.18	122.92
31	G	603	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
48	s	621	LUT	C18-C5-C6	-3.38	120.73	124.53
47	N1	601	CHL	C2C-C3C-C4C	3.38	108.90	106.49
31	R	604	CLA	C2C-C1C-NC	3.38	113.14	109.97
31	D1	403	CLA	C1-C2-C3	-3.38	120.20	126.04
33	d1	404	BCR	C33-C5-C4	3.38	120.11	113.62
31	S1	605	CLA	C2C-C1C-NC	3.38	113.14	109.97
31	C	509	CLA	C2C-C1C-NC	3.38	113.14	109.97
31	r	609	CLA	C1-C2-C3	-3.38	120.20	126.04
31	y	608	CLA	C1-C2-C3	-3.38	121.29	126.75
33	C	514	BCR	C15-C14-C13	-3.38	122.49	127.31
33	B	618	BCR	C33-C5-C6	-3.38	120.74	124.53
31	C1	512	CLA	C2C-C1C-NC	3.38	113.14	109.97
33	d	404	BCR	C33-C5-C4	3.38	120.10	113.62
31	N1	614	CLA	CHD-C1D-ND	-3.38	121.35	124.45
31	B	602	CLA	C2C-C1C-NC	3.38	113.13	109.97
31	B1	603	CLA	C2C-C1C-NC	3.38	113.13	109.97
31	C1	504	CLA	CHD-C1D-ND	-3.37	121.35	124.45
31	B1	616	CLA	C1-C2-C3	-3.37	120.21	126.04
31	n	611	CLA	CMA-C3A-C4A	3.37	120.84	111.77
31	s1	603	CLA	C2C-C1C-NC	3.37	113.13	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	604	CLA	CHD-C1D-ND	-3.37	121.36	124.45
31	n1	603	CLA	C2C-C1C-NC	3.37	113.13	109.97
31	c1	510	CLA	C2C-C1C-NC	3.37	113.13	109.97
31	B	616	CLA	C1-C2-C3	-3.37	120.21	126.04
31	c	504	CLA	C2D-C1D-ND	3.37	112.59	110.10
31	s	610	CLA	CAA-C2A-C3A	-3.37	103.55	112.78
31	A1	406	CLA	CMA-C3A-C4A	3.37	120.83	111.77
33	c1	515	BCR	C33-C5-C6	-3.37	120.74	124.53
31	R1	604	CLA	C2C-C1C-NC	3.37	113.13	109.97
31	n1	613	CLA	CMA-C3A-C4A	3.37	120.83	111.77
31	c	506	CLA	C2C-C1C-NC	3.37	113.13	109.97
31	b	603	CLA	C1-C2-C3	-3.37	120.22	126.04
47	y	609	CHL	CHD-C1D-ND	-3.37	121.36	124.45
50	r1	622	NEX	C19-C9-C10	-3.37	118.21	122.92
31	B	612	CLA	C2D-C1D-ND	3.37	112.58	110.10
31	S1	605	CLA	C1-C2-C3	-3.37	121.31	126.75
47	R	607	CHL	CHD-C1D-ND	-3.36	121.36	124.45
31	B	610	CLA	C1-C2-C3	-3.36	120.22	126.04
31	G	603	CLA	CMA-C3A-C4A	3.36	120.81	111.77
48	s	621	LUT	C15-C14-C13	-3.36	122.51	127.31
31	S1	614	CLA	CHD-C1D-ND	-3.36	121.36	124.45
31	G1	611	CLA	CHD-C1D-ND	-3.36	121.37	124.45
40	C1	519	DGD	O1G-C1A-C2A	3.36	122.45	111.91
47	g	607	CHL	CHD-C1D-ND	-3.36	121.37	124.45
31	N	612	CLA	C2C-C1C-NC	3.35	113.11	109.97
48	Y	621	LUT	C22-C23-C24	-3.35	107.92	111.74
31	G	603	CLA	CHD-C1D-ND	-3.35	121.37	124.45
47	g	606	CHL	C3C-C4C-NC	-3.35	106.81	110.57
32	a	409	PHO	CMB-C2B-C3B	3.35	130.95	124.68
33	A1	411	BCR	C38-C26-C25	-3.35	120.77	124.53
31	C1	511	CLA	C2C-C1C-NC	3.35	113.11	109.97
47	S	601	CHL	C2C-C3C-C4C	3.35	108.88	106.49
31	s	603	CLA	C2C-C1C-NC	3.35	113.11	109.97
31	Y1	608	CLA	C2C-C1C-NC	3.35	113.11	109.97
31	B	604	CLA	CMB-C2B-C3B	3.34	130.94	124.68
33	B1	618	BCR	C33-C5-C6	-3.34	120.77	124.53
33	d1	404	BCR	C34-C9-C10	-3.34	118.24	122.92
31	B	612	CLA	CMB-C2B-C3B	3.34	130.93	124.68
48	n	621	LUT	C18-C5-C6	-3.34	120.77	124.53
46	h1	101	RRX	C34-C9-C8	3.34	123.34	118.08
47	n	601	CHL	C3C-C4C-NC	-3.34	106.82	110.57
31	b1	603	CLA	O2A-CGA-CBA	3.34	122.39	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	507	CLA	CHD-C1D-ND	-3.34	121.38	124.45
47	Y1	607	CHL	C2C-C3C-C4C	3.34	108.87	106.49
48	n1	620	LUT	C7-C8-C9	-3.34	121.19	126.23
48	Y	620	LUT	C18-C5-C6	-3.34	120.78	124.53
31	y1	610	CLA	C1-C2-C3	-3.34	120.27	126.04
31	a	410	CLA	CMA-C3A-C4A	3.34	120.75	111.77
46	H1	101	RRX	C23-C22-C21	-3.34	113.82	118.94
47	G	606	CHL	CHD-C1D-ND	-3.34	121.39	124.45
50	N	623	NEX	C40-C33-C34	-3.34	118.25	122.92
47	y1	607	CHL	CHB-C4A-NA	3.34	129.13	124.51
47	y	607	CHL	CHD-C1D-ND	-3.34	121.39	124.45
46	h	101	RRX	C7-C8-C9	-3.34	121.19	126.23
47	y	601	CHL	CHD-C1D-ND	-3.34	121.39	124.45
31	C	513	CLA	CMB-C2B-C3B	3.34	130.92	124.68
31	r1	604	CLA	C2C-C1C-NC	3.33	113.10	109.97
50	R1	622	NEX	C2-C1-C6	3.33	112.45	109.21
31	b1	611	CLA	C2D-C1D-ND	3.33	112.56	110.10
31	y1	602	CLA	C1-C2-C3	-3.33	120.28	126.04
47	g	601	CHL	C3C-C4C-NC	-3.33	106.83	110.57
31	G	613	CLA	C1-C2-C3	-3.33	120.28	126.04
47	n	607	CHL	CHD-C1D-ND	-3.33	121.39	124.45
31	r1	609	CLA	C2C-C1C-NC	3.33	113.09	109.97
31	r	608	CLA	CHD-C1D-ND	-3.33	121.39	124.45
46	H	101	RRX	C4-C5-C6	-3.33	117.90	122.73
31	b1	611	CLA	C2C-C1C-NC	3.33	113.09	109.97
31	y	602	CLA	CMC-C2C-C1C	3.33	130.11	125.04
31	D1	402	CLA	CHD-C1D-ND	-3.33	121.40	124.45
31	c	503	CLA	CMA-C3A-C4A	3.33	120.72	111.77
50	S	622	NEX	C5-C4-C3	3.33	115.68	111.75
31	S	603	CLA	C2C-C1C-NC	3.33	113.09	109.97
31	s	610	CLA	CHD-C1D-ND	-3.33	121.40	124.45
31	C1	512	CLA	CHD-C1D-ND	-3.33	121.40	124.45
31	S1	604	CLA	C2C-C1C-NC	3.33	113.09	109.97
31	n1	604	CLA	C1-C2-C3	-3.33	120.29	126.04
47	G	608	CHL	C2C-C3C-C4C	3.32	108.86	106.49
47	g	601	CHL	C2C-C3C-C4C	3.32	108.86	106.49
31	g	613	CLA	C2D-C1D-ND	3.32	112.55	110.10
31	N1	611	CLA	C2C-C1C-NC	3.32	113.08	109.97
47	G	607	CHL	CHD-C1D-ND	-3.32	121.40	124.45
56	r1	626	ERG	C1-C10-C5	3.32	114.83	108.75
47	R	607	CHL	C2C-C3C-C4C	3.32	108.86	106.49
31	S1	614	CLA	C2C-C1C-NC	3.32	113.08	109.97

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	609	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
31	S	613	CLA	CMA-C3A-C4A	3.32	120.69	111.77
31	C	504	CLA	C2D-C1D-ND	3.32	112.55	110.10
31	Y	612	CLA	C2D-C1D-ND	3.32	112.55	110.10
31	B1	612	CLA	C2D-C1D-ND	3.32	112.55	110.10
31	n	602	CLA	C1-C2-C3	-3.32	120.31	126.04
31	R1	612	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	c	509	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
31	n	603	CLA	C2C-C1C-NC	3.32	113.08	109.97
47	Y1	607	CHL	C3C-C4C-NC	-3.32	106.85	110.57
31	R1	610	CLA	C2D-C1D-ND	3.32	112.55	110.10
31	s	605	CLA	C2C-C1C-NC	3.31	113.08	109.97
31	Y	613	CLA	CMA-C3A-C4A	3.31	120.68	111.77
31	g	602	CLA	C2D-C1D-ND	3.31	112.55	110.10
31	G1	603	CLA	C2C-C1C-NC	3.31	113.08	109.97
50	S1	623	NEX	C27-C28-C29	-3.31	120.39	125.53
31	y	612	CLA	C2C-C1C-NC	3.31	113.07	109.97
50	N1	623	NEX	C39-C29-C30	-3.31	118.29	122.92
31	r1	604	CLA	CHD-C1D-ND	-3.31	121.41	124.45
49	N1	622	XAT	C6-C7-C8	-3.31	119.00	125.99
31	G	604	CLA	C2C-C1C-NC	3.31	113.07	109.97
31	y1	611	CLA	C2C-C1C-NC	3.31	113.07	109.97
47	y1	609	CHL	C2C-C3C-C4C	3.31	108.85	106.49
31	b1	607	CLA	CHD-C1D-ND	-3.31	121.42	124.45
33	C	515	BCR	C33-C5-C4	3.31	119.97	113.62
50	G1	623	NEX	C17-C1-C6	-3.31	107.51	110.47
47	R	606	CHL	CHD-C1D-ND	-3.30	121.42	124.45
31	B1	612	CLA	CMB-C2B-C3B	3.30	130.86	124.68
31	N	610	CLA	O2A-CGA-CBA	3.30	122.28	111.91
31	B1	608	CLA	C2C-C1C-NC	3.30	113.07	109.97
31	b1	616	CLA	C2C-C1C-NC	3.30	113.07	109.97
31	D	402	CLA	CHD-C1D-ND	-3.30	121.42	124.45
32	a1	408	PHO	CMB-C2B-C3B	3.30	130.86	124.68
31	G1	602	CLA	C1-C2-C3	-3.30	120.33	126.04
31	R1	608	CLA	CHD-C1D-ND	-3.30	121.42	124.45
47	s	607	CHL	CHD-C1D-ND	-3.30	121.42	124.45
31	B	612	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
31	c	506	CLA	CHD-C1D-ND	-3.30	121.42	124.45
33	B1	618	BCR	C15-C14-C13	-3.30	122.60	127.31
50	s1	623	NEX	C1-C2-C3	3.30	121.10	113.64
31	y	602	CLA	C1-C2-C3	-3.30	120.33	126.04
31	s1	613	CLA	CMA-C3A-C4A	3.30	120.64	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	614	CLA	C2C-C1C-NC	3.30	113.06	109.97
31	s1	611	CLA	C2C-C1C-NC	3.30	113.06	109.97
50	g	623	NEX	C27-C28-C29	-3.30	120.41	125.53
31	C	503	CLA	CHD-C1D-ND	-3.30	121.42	124.45
31	B1	602	CLA	C2C-C1C-NC	3.30	113.06	109.97
31	G	614	CLA	CHD-C1D-ND	-3.30	121.42	124.45
31	g1	610	CLA	CHD-C1D-ND	-3.30	121.42	124.45
31	y	613	CLA	CHD-C1D-ND	-3.29	121.43	124.45
48	N1	621	LUT	C31-C30-C29	-3.29	122.61	127.31
31	B	611	CLA	C1-C2-C3	-3.29	120.34	126.04
48	G1	621	LUT	C18-C5-C6	-3.29	120.83	124.53
31	d1	403	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	g1	611	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	b	611	CLA	C2D-C1D-ND	3.29	112.53	110.10
31	b1	612	CLA	C2D-C1D-ND	3.29	112.53	110.10
50	g	623	NEX	O24-C25-C38	-3.29	111.11	115.06
31	C1	502	CLA	C2C-C1C-NC	3.29	113.06	109.97
31	c1	506	CLA	C2C-C1C-NC	3.29	113.06	109.97
56	r1	626	ERG	C18-C13-C14	-3.29	104.91	110.24
47	S	606	CHL	C2C-C3C-C4C	3.29	108.84	106.49
31	y1	602	CLA	CMB-C2B-C3B	3.29	130.84	124.68
49	n1	622	XAT	C38-C25-C26	-3.29	116.74	122.26
31	y	611	CLA	C2C-C1C-NC	3.29	113.06	109.97
31	g1	603	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	b	607	CLA	C2C-C1C-NC	3.29	113.05	109.97
47	N1	607	CHL	CHD-C1D-ND	-3.29	121.43	124.45
31	y1	603	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	N1	613	CLA	C2C-C1C-NC	3.29	113.05	109.97
49	g1	622	XAT	C7-C8-C9	-3.29	120.43	125.53
31	Y1	612	CLA	C2C-C1C-NC	3.28	113.05	109.97
47	G	607	CHL	C2C-C3C-C4C	3.28	108.83	106.49
31	C	508	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
31	r	608	CLA	C2C-C1C-NC	3.28	113.05	109.97
31	y	610	CLA	CHD-C1D-ND	-3.28	121.44	124.45
31	C	507	CLA	C2C-C1C-NC	3.28	113.05	109.97
31	S	613	CLA	C2D-C1D-ND	3.28	112.52	110.10
50	r1	622	NEX	C27-C28-C29	-3.28	120.44	125.53
31	r1	610	CLA	C1-C2-C3	-3.28	120.37	126.04
50	S	622	NEX	C31-C30-C29	3.28	131.99	127.31
47	r	607	CHL	C2C-C3C-C4C	3.28	108.83	106.49
33	a1	411	BCR	C33-C5-C6	-3.28	120.84	124.53
31	A1	406	CLA	CHD-C1D-ND	-3.28	121.44	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g1	610	CLA	C1-C2-C3	-3.28	120.37	126.04
31	s1	603	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
31	n	603	CLA	CHD-C1D-ND	-3.28	121.44	124.45
31	D	403	CLA	CHD-C1D-ND	-3.28	121.44	124.45
31	a1	406	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
31	D	402	CLA	C1D-ND-C4D	-3.28	104.01	106.33
31	n1	610	CLA	CHD-C1D-ND	-3.28	121.44	124.45
31	b	606	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
31	R	612	CLA	C2C-C1C-NC	3.27	113.04	109.97
31	B	607	CLA	CMA-C3A-C4A	3.27	120.57	111.77
31	s1	612	CLA	CHD-C1D-ND	-3.27	121.44	124.45
33	C1	514	BCR	C36-C18-C17	-3.27	118.34	122.92
47	N	601	CHL	C2C-C3C-C4C	3.27	108.82	106.49
47	y	607	CHL	C4A-NA-C1A	3.27	108.18	106.71
49	r1	621	XAT	C40-C33-C34	-3.27	118.34	122.92
31	Y	604	CLA	CHD-C1D-ND	-3.27	121.45	124.45
31	S1	602	CLA	C2D-C1D-ND	3.27	112.51	110.10
47	Y1	606	CHL	C2C-C3C-C4C	3.27	108.82	106.49
31	B1	606	CLA	CHD-C1D-ND	-3.27	121.45	124.45
47	G1	606	CHL	CHD-C1D-ND	-3.27	121.45	124.45
47	G	606	CHL	C3C-C4C-NC	-3.27	106.90	110.57
47	G1	607	CHL	CMA-C3A-C4A	3.27	120.56	111.77
31	N	603	CLA	C2C-C1C-NC	3.27	113.03	109.97
31	a	406	CLA	C2C-C1C-NC	3.27	113.03	109.97
31	y	608	CLA	CHD-C1D-ND	-3.27	121.45	124.45
31	y	602	CLA	C1D-ND-C4D	-3.27	104.01	106.33
46	h1	101	RRX	C33-C5-C6	-3.27	120.86	124.53
31	c	509	CLA	C1-C2-C3	-3.27	120.39	126.04
31	s1	610	CLA	C1-C2-C3	-3.27	120.39	126.04
31	B1	608	CLA	CHD-C1D-ND	-3.27	121.45	124.45
31	b1	616	CLA	C1-C2-C3	-3.27	120.39	126.04
47	G	609	CHL	CHD-C4C-C3C	3.27	129.64	124.84
31	d1	402	CLA	C2D-C1D-ND	3.26	112.51	110.10
47	N1	606	CHL	C3C-C4C-NC	-3.26	106.91	110.57
31	c	504	CLA	CHD-C1D-ND	-3.26	121.45	124.45
33	b1	618	BCR	C1-C6-C5	-3.26	118.02	122.61
48	y	620	LUT	C35-C15-C14	-3.26	116.79	123.47
31	c	512	CLA	C2C-C1C-NC	3.26	113.03	109.97
31	N1	612	CLA	C2C-C1C-NC	3.26	113.03	109.97
31	r1	612	CLA	C2C-C1C-NC	3.26	113.03	109.97
56	r1	626	ERG	C16-C17-C13	3.26	107.77	103.84
50	y	623	NEX	C17-C1-C6	-3.26	107.56	110.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	n	605	CHL	C3C-C4C-NC	-3.26	106.92	110.57
47	r	607	CHL	C3C-C4C-NC	-3.26	106.92	110.57
31	s	614	CLA	CHD-C1D-ND	-3.26	121.46	124.45
37	b	620	C7Z	C8-C7-C6	-3.26	118.05	127.20
31	y	603	CLA	C2C-C1C-NC	3.26	113.03	109.97
33	c	516	BCR	C34-C9-C10	-3.26	118.36	122.92
31	A	406	CLA	CHD-C1D-ND	-3.26	121.46	124.45
47	Y1	607	CHL	CHD-C1D-ND	-3.26	121.46	124.45
31	R1	610	CLA	CMB-C2B-C3B	3.26	130.77	124.68
47	R1	606	CHL	CHD-C1D-ND	-3.26	121.46	124.45
31	C1	513	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
48	N1	620	LUT	C15-C14-C13	-3.26	122.66	127.31
50	g1	623	NEX	C19-C9-C10	-3.26	118.36	122.92
31	B	617	CLA	C2C-C1C-NC	3.25	113.02	109.97
47	Y1	606	CHL	CHD-C1D-ND	-3.25	121.46	124.45
47	n1	609	CHL	CMA-C3A-C4A	3.25	120.52	111.77
31	G1	602	CLA	C1D-ND-C4D	-3.25	104.02	106.33
48	g1	621	LUT	C15-C14-C13	-3.25	122.67	127.31
31	d	402	CLA	C1-C2-C3	-3.25	120.42	126.04
31	a	406	CLA	CMB-C2B-C3B	3.25	130.76	124.68
37	B1	620	C7Z	C18-C5-C4	3.25	120.38	114.36
48	g	620	LUT	C15-C14-C13	-3.25	122.67	127.31
31	c	504	CLA	O2A-CGA-CBA	3.25	122.11	111.91
31	N	614	CLA	C2C-C1C-NC	3.25	113.02	109.97
37	b	620	C7Z	C31-C30-C29	-3.25	122.67	127.31
31	s	612	CLA	CHD-C1D-ND	-3.25	121.47	124.45
43	d1	401	BCT	O3-C-O1	-3.25	111.12	119.55
44	d1	405	PL9	C36-C34-C33	-3.25	114.55	121.12
31	B	612	CLA	CMA-C3A-C4A	3.25	120.50	111.77
47	g	608	CHL	CMA-C3A-C4A	3.25	120.50	111.77
31	S1	617	CLA	C2C-C1C-NC	3.25	113.01	109.97
31	r	610	CLA	CMA-C3A-C4A	3.24	120.49	111.77
50	r	623	NEX	C27-C28-C29	-3.24	120.50	125.53
33	C1	515	BCR	C33-C5-C4	3.24	119.84	113.62
31	y	603	CLA	C2D-C1D-ND	3.24	112.49	110.10
31	n1	602	CLA	CHD-C1D-ND	-3.24	121.47	124.45
31	g	614	CLA	C2C-C1C-NC	3.24	113.01	109.97
31	b	615	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
31	g	604	CLA	CHD-C1D-ND	-3.24	121.48	124.45
47	n1	609	CHL	C3C-C4C-NC	-3.24	106.94	110.57
31	S1	603	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
31	B	603	CLA	C2C-C1C-NC	3.24	113.01	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r	622	XAT	C20-C13-C14	-3.24	118.39	122.92
41	s	624	LHG	C5-O7-C7	-3.24	109.82	117.79
47	s1	607	CHL	C2C-C3C-C4C	3.24	108.80	106.49
50	G1	623	NEX	C16-C1-C6	-3.24	107.58	110.47
47	S	608	CHL	CMA-C3A-C4A	3.24	120.47	111.77
46	h	101	RRX	C15-C16-C17	-3.24	116.85	123.47
31	s1	604	CLA	C1-C2-C3	-3.23	120.45	126.04
50	g1	623	NEX	C38-C25-C26	-3.23	116.84	122.26
47	n	607	CHL	C1-O2A-CGA	3.23	124.93	116.44
31	n1	611	CLA	C2D-C1D-ND	3.23	112.49	110.10
31	A	405	CLA	CMB-C2B-C3B	3.23	130.73	124.68
47	N	601	CHL	C3C-C4C-NC	-3.23	106.95	110.57
47	G1	606	CHL	C3C-C4C-NC	-3.23	106.95	110.57
31	Y	614	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	B1	617	CLA	C2C-C1C-NC	3.23	113.00	109.97
47	g1	606	CHL	C2C-C3C-C4C	3.23	108.79	106.49
31	R	609	CLA	CHD-C1D-ND	-3.23	121.49	124.45
31	N1	611	CLA	CHD-C1D-ND	-3.23	121.49	124.45
31	B1	611	CLA	C2D-C1D-ND	3.23	112.48	110.10
31	b1	605	CLA	C2D-C1D-ND	3.23	112.48	110.10
31	b1	605	CLA	O2A-CGA-CBA	3.23	122.04	111.91
31	b1	614	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	y1	603	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	B1	603	CLA	CHD-C1D-ND	-3.23	121.49	124.45
31	y1	612	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	b	606	CLA	CHD-C1D-ND	-3.23	121.49	124.45
31	y1	610	CLA	CHD-C1D-ND	-3.23	121.49	124.45
47	g1	605	CHL	CHD-C1D-ND	-3.23	121.49	124.45
48	s	621	LUT	C7-C8-C9	-3.23	121.36	126.23
31	b1	607	CLA	CMA-C3A-C4A	3.23	120.44	111.77
31	N	604	CLA	CHD-C1D-ND	-3.23	121.49	124.45
47	n1	608	CHL	C2C-C3C-C4C	3.23	108.79	106.49
31	b	609	CLA	CMB-C2B-C3B	3.23	130.71	124.68
31	c1	512	CLA	C2C-C1C-NC	3.22	112.99	109.97
31	Y	603	CLA	CHD-C1D-ND	-3.22	121.49	124.45
49	G1	622	XAT	C38-C25-C26	-3.22	116.86	122.26
33	c1	514	BCR	C38-C26-C25	-3.22	120.91	124.53
31	c	502	CLA	C2D-C1D-ND	3.22	112.48	110.10
33	d	404	BCR	C27-C26-C25	-3.22	118.05	122.73
47	Y1	606	CHL	CMA-C3A-C4A	3.22	120.43	111.77
31	R1	612	CLA	CHD-C1D-ND	-3.22	121.49	124.45
31	Y1	604	CLA	CHD-C1D-ND	-3.22	121.49	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	609	CLA	C2C-C1C-NC	3.22	112.99	109.97
31	s1	617	CLA	C1-C2-C3	-3.22	121.54	126.75
33	c	514	BCR	C33-C5-C6	-3.22	120.91	124.53
31	b	603	CLA	CHD-C1D-ND	-3.22	121.50	124.45
31	S	613	CLA	C2C-C1C-NC	3.22	112.99	109.97
48	Y1	621	LUT	C11-C10-C9	-3.22	122.72	127.31
31	B1	609	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
31	N	612	CLA	CMA-C3A-C4A	3.22	120.42	111.77
31	B	604	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
31	B	603	CLA	CHD-C1D-ND	-3.22	121.50	124.45
33	B	619	BCR	C37-C22-C21	-3.22	118.42	122.92
31	b	611	CLA	CMA-C3A-C4A	3.22	120.42	111.77
47	Y	606	CHL	CHD-C1D-ND	-3.22	121.50	124.45
47	y	606	CHL	CMA-C3A-C4A	3.22	120.42	111.77
33	A1	411	BCR	C33-C5-C4	3.22	119.79	113.62
31	G1	613	CLA	CHD-C1D-ND	-3.22	121.50	124.45
31	B	613	CLA	C2C-C1C-NC	3.22	112.98	109.97
31	b	602	CLA	CMA-C3A-C4A	3.21	120.41	111.77
31	s1	609	CLA	C2C-C1C-NC	3.21	112.98	109.97
47	G	606	CHL	CMA-C3A-C4A	3.21	120.41	111.77
31	G	613	CLA	CHD-C1D-ND	-3.21	121.50	124.45
48	y	621	LUT	C18-C5-C6	-3.21	120.92	124.53
47	N	608	CHL	CMA-C3A-C4A	3.21	120.41	111.77
31	a	410	CLA	C2C-C1C-NC	3.21	112.98	109.97
31	C1	504	CLA	C2C-C1C-NC	3.21	112.98	109.97
48	y1	621	LUT	C3-C4-C5	-3.21	105.46	111.85
31	C1	506	CLA	CHD-C1D-ND	-3.21	121.50	124.45
47	G	601	CHL	C3C-C4C-NC	-3.21	106.97	110.57
31	B	610	CLA	C2C-C1C-NC	3.21	112.98	109.97
31	s	611	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	b1	608	CLA	C2C-C1C-NC	3.21	112.98	109.97
31	S	604	CLA	CHD-C1D-ND	-3.21	121.51	124.45
31	c1	504	CLA	CHD-C1D-ND	-3.21	121.51	124.45
47	y	605	CHL	CHD-C1D-ND	-3.21	121.51	124.45
31	s1	612	CLA	C2D-C1D-ND	3.21	112.47	110.10
48	G	621	LUT	C7-C8-C9	-3.21	121.39	126.23
31	C	509	CLA	CHD-C1D-ND	-3.21	121.51	124.45
47	Y1	607	CHL	C4A-NA-C1A	3.21	108.15	106.71
31	N1	614	CLA	C2D-C1D-ND	3.21	112.47	110.10
48	G	620	LUT	C18-C5-C6	-3.20	120.93	124.53
31	c1	501	CLA	CHD-C1D-ND	-3.20	121.51	124.45
31	b1	603	CLA	CHD-C1D-ND	-3.20	121.51	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	607	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
31	y	613	CLA	C1-C2-C3	-3.20	120.50	126.04
31	b1	611	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
47	G	607	CHL	C3C-C4C-NC	-3.20	106.98	110.57
31	N	611	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	A1	406	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
33	B1	619	BCR	C33-C5-C6	-3.20	120.93	124.53
31	C	506	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	R	611	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	r	602	CLA	CMB-C2B-C3B	3.20	130.66	124.68
47	G1	608	CHL	CMA-C3A-C4A	3.20	120.37	111.77
48	S1	621	LUT	C11-C10-C9	-3.20	122.75	127.31
31	A	405	CLA	CHD-C1D-ND	-3.20	121.52	124.45
31	c	507	CLA	CHD-C1D-ND	-3.20	121.52	124.45
31	n	611	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	S1	610	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	b	612	CLA	CMB-C2B-C3B	3.20	130.66	124.68
31	g	611	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	n	610	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
31	s1	602	CLA	C2D-C1D-ND	3.20	112.46	110.10
47	G	608	CHL	C3C-C4C-NC	-3.19	106.99	110.57
50	S1	623	NEX	C31-C30-C29	3.19	131.87	127.31
31	A1	410	CLA	CMA-C3A-C4A	3.19	120.36	111.77
47	r1	607	CHL	CMA-C3A-C4A	3.19	120.36	111.77
47	R1	607	CHL	C2C-C3C-C4C	3.19	108.77	106.49
31	a1	410	CLA	CMB-C2B-C3B	3.19	130.65	124.68
50	G	623	NEX	C1-C2-C3	3.19	120.85	113.64
47	N	606	CHL	C3C-C4C-NC	-3.19	106.99	110.57
31	R	612	CLA	CHD-C1D-ND	-3.19	121.52	124.45
31	Y1	611	CLA	C2C-C1C-NC	3.19	112.96	109.97
47	Y	607	CHL	C2C-C3C-C4C	3.19	108.76	106.49
31	g	603	CLA	CMA-C3A-C4A	3.19	120.35	111.77
31	C	513	CLA	CHD-C1D-ND	-3.19	121.52	124.45
31	Y1	603	CLA	CMA-C3A-C4A	3.19	120.34	111.77
49	Y	622	XAT	C6-C7-C8	-3.19	119.25	125.99
31	C1	513	CLA	C2D-C1D-ND	3.19	112.45	110.10
31	G1	603	CLA	C1-C2-C3	-3.19	120.53	126.04
31	d1	403	CLA	C2C-C1C-NC	3.19	112.96	109.97
48	n1	620	LUT	C18-C5-C6	-3.19	120.95	124.53
49	N1	622	XAT	C7-C8-C9	-3.19	120.58	125.53
31	R	603	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	r	602	CLA	CHD-C1D-ND	-3.19	121.53	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	R	621	XAT	C26-C27-C28	-3.18	119.26	125.99
31	b1	604	CLA	C2D-C1D-ND	3.18	112.45	110.10
31	d1	403	CLA	CMB-C2B-C3B	3.18	130.63	124.68
31	n1	614	CLA	CHD-C1D-ND	-3.18	121.53	124.45
41	L	101	LHG	O7-C7-C8	3.18	118.36	111.50
47	n	606	CHL	CMA-C3A-C4A	3.18	120.33	111.77
31	c1	505	CLA	C2C-C1C-NC	3.18	112.95	109.97
31	r	610	CLA	C2D-C1D-ND	3.18	112.45	110.10
31	s1	617	CLA	C2D-C1D-ND	3.18	112.45	110.10
31	n	613	CLA	CHD-C1D-ND	-3.18	121.53	124.45
31	n	614	CLA	CHD-C1D-ND	-3.18	121.53	124.45
47	r1	607	CHL	CHD-C1D-ND	-3.18	121.53	124.45
31	y1	603	CLA	CMA-C3A-C4A	3.18	120.32	111.77
50	g1	623	NEX	C11-C10-C9	3.18	131.85	127.31
31	s1	605	CLA	C1-C2-C3	-3.18	121.61	126.75
33	a1	411	BCR	C23-C24-C25	-3.18	118.28	127.20
31	n1	612	CLA	C2C-C1C-NC	3.18	112.95	109.97
47	G	605	CHL	C2C-C3C-C4C	3.18	108.75	106.49
31	Y1	613	CLA	C1C-C2C-C3C	-3.18	103.62	106.96
31	N1	603	CLA	CHD-C1D-ND	-3.18	121.53	124.45
47	N	607	CHL	C2C-C3C-C4C	3.18	108.75	106.49
31	R	610	CLA	C1-C2-C3	-3.18	120.55	126.04
31	S1	603	CLA	CMA-C3A-C4A	3.17	120.31	111.77
47	s1	607	CHL	CMA-C3A-C4A	3.17	120.31	111.77
31	C	501	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	c	510	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	C	506	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
43	D	401	BCT	O3-C-O1	-3.17	111.31	119.55
31	Y1	611	CLA	CHD-C1D-ND	-3.17	121.54	124.45
47	N1	609	CHL	CMA-C3A-C4A	3.17	120.30	111.77
31	G1	610	CLA	C2D-C1D-ND	3.17	112.44	110.10
31	C	510	CLA	C2C-C1C-NC	3.17	112.94	109.97
47	n1	601	CHL	C3C-C4C-NC	-3.17	107.01	110.57
31	Y	603	CLA	C2D-C1D-ND	3.17	112.44	110.10
44	d	405	PL9	C7-C3-C2	-3.17	119.13	123.30
31	y1	604	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	c1	512	CLA	CMB-C2B-C3B	3.17	130.61	124.68
31	c	505	CLA	CMA-C3A-C4A	3.17	120.29	111.77
31	c1	501	CLA	CMA-C3A-C4A	3.17	120.29	111.77
31	C1	505	CLA	C2C-C1C-NC	3.17	112.94	109.97
31	G	602	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	S	605	CLA	C2C-C1C-NC	3.17	112.94	109.97

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	602	CLA	CHD-C1D-ND	-3.17	121.54	124.45
49	g1	622	XAT	C38-C25-C26	-3.17	116.95	122.26
48	g	620	LUT	C31-C30-C29	-3.17	122.79	127.31
31	S1	617	CLA	C2D-C1D-ND	3.17	112.44	110.10
31	b	608	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	c	501	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	b	612	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
31	C1	507	CLA	C2C-C1C-NC	3.17	112.94	109.97
47	y1	605	CHL	CMA-C3A-C4A	3.17	120.28	111.77
47	Y	609	CHL	C3C-C4C-NC	-3.17	107.02	110.57
31	r	611	CLA	C2C-C1C-NC	3.17	112.94	109.97
31	R1	604	CLA	CMA-C3A-C4A	3.17	120.28	111.77
47	Y1	605	CHL	CMA-C3A-C4A	3.17	120.28	111.77
31	Y1	614	CLA	C2C-C1C-NC	3.16	112.94	109.97
47	n	607	CHL	C2C-C3C-C4C	3.16	108.75	106.49
31	a	407	CLA	CMA-C3A-C4A	3.16	120.28	111.77
47	y1	609	CHL	C3C-C4C-NC	-3.16	107.02	110.57
47	Y	607	CHL	CHD-C1D-ND	-3.16	121.55	124.45
33	C	516	BCR	C34-C9-C10	-3.16	118.49	122.92
31	y1	604	CLA	C2C-C1C-NC	3.16	112.94	109.97
47	N1	608	CHL	CMA-C3A-C4A	3.16	120.28	111.77
31	Y	610	CLA	C1-C2-C3	-3.16	120.57	126.04
47	Y1	605	CHL	C2C-C3C-C4C	3.16	108.74	106.49
31	c1	513	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
31	B	616	CLA	C2C-C1C-NC	3.16	112.93	109.97
47	n1	608	CHL	C1-O2A-CGA	3.16	124.74	116.44
33	b	619	BCR	C19-C18-C17	3.16	123.79	118.94
31	c	504	CLA	C2C-C1C-NC	3.16	112.93	109.97
31	a	406	CLA	C1-C2-C3	-3.16	120.58	126.04
48	y1	620	LUT	C11-C10-C9	-3.16	122.80	127.31
33	B1	619	BCR	C4-C5-C6	-3.16	118.14	122.73
31	a1	405	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	b	605	CLA	C1-C2-C3	-3.16	120.58	126.04
33	a	411	BCR	C33-C5-C6	-3.16	120.98	124.53
33	b	619	BCR	C33-C5-C4	3.16	119.69	113.62
47	S	607	CHL	C2C-C3C-C4C	3.16	108.74	106.49
49	Y	622	XAT	C38-C25-C26	-3.16	116.97	122.26
47	Y	601	CHL	CMA-C3A-C4A	3.16	120.26	111.77
31	Y	602	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
31	s	604	CLA	C1-C2-C3	-3.16	120.58	126.04
31	Y1	604	CLA	C2C-C1C-NC	3.16	112.93	109.97
31	g1	614	CLA	C2C-C1C-NC	3.16	112.93	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	G1	605	CHL	CMA-C3A-C4A	3.16	120.26	111.77
31	b	607	CLA	CMD-C2D-C3D	-3.16	120.35	127.61
31	Y1	602	CLA	C1-C2-C3	-3.16	120.58	126.04
47	y	607	CHL	C2C-C3C-C4C	3.16	108.74	106.49
47	g1	607	CHL	C4A-NA-C1A	3.16	108.12	106.71
31	n	613	CLA	C2D-C1D-ND	3.15	112.43	110.10
31	B1	614	CLA	CHD-C1D-ND	-3.15	121.56	124.45
31	n1	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
31	S1	611	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
48	G	621	LUT	C18-C5-C6	-3.15	120.99	124.53
33	C1	517	BCR	C23-C24-C25	-3.15	118.35	127.20
31	r	613	CLA	CMA-C3A-C4A	3.15	120.25	111.77
49	n1	622	XAT	O24-C25-C24	3.15	115.75	113.38
31	s	617	CLA	C2C-C1C-NC	3.15	112.92	109.97
47	N	607	CHL	C3C-C4C-NC	-3.15	107.04	110.57
31	A	407	CLA	CHD-C1D-ND	-3.15	121.56	124.45
47	g	605	CHL	C3C-C4C-NC	-3.15	107.04	110.57
47	y	609	CHL	C2C-C3C-C4C	3.15	108.73	106.49
31	g	603	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
31	C	508	CLA	CMB-C2B-C3B	3.15	130.57	124.68
31	Y1	613	CLA	CMA-C3A-C4A	3.15	120.23	111.77
47	n	608	CHL	CMA-C3A-C4A	3.15	120.23	111.77
45	F	101	HEM	C1B-NB-C4B	3.15	108.32	105.07
40	C	523	DGD	O1G-C1A-C2A	3.14	121.78	111.91
31	A1	407	CLA	CMA-C3A-C4A	3.14	120.22	111.77
31	B	614	CLA	C2D-C1D-ND	3.14	112.42	110.10
31	C1	512	CLA	C2D-C1D-ND	3.14	112.42	110.10
31	s1	603	CLA	CMA-C3A-C4A	3.14	120.22	111.77
47	S1	607	CHL	C2C-C3C-C4C	3.14	108.73	106.49
31	B	614	CLA	C2C-C1C-NC	3.14	112.92	109.97
31	S1	613	CLA	CMA-C3A-C4A	3.14	120.22	111.77
31	A1	410	CLA	C2D-C1D-ND	3.14	112.42	110.10
31	Y	608	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	b	614	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	a1	407	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	s1	611	CLA	C2D-C1D-ND	3.14	112.42	110.10
31	R1	612	CLA	C1-C2-C3	-3.14	120.61	126.04
31	n1	604	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	R1	610	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	N	613	CLA	O2A-CGA-CBA	3.14	121.76	111.91
31	S	617	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	b1	606	CLA	C2C-C1C-NC	3.14	112.91	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	614	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	C1	503	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	R	611	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	b1	603	CLA	CMA-C3A-C4A	3.14	120.20	111.77
31	s1	603	CLA	C1-C2-C3	-3.14	120.62	126.04
31	S	612	CLA	C2D-C1D-ND	3.14	112.42	110.10
49	N	622	XAT	C38-C25-C26	-3.14	117.00	122.26
31	Y1	602	CLA	CMA-C3A-C4A	3.14	120.20	111.77
47	n	607	CHL	CMA-C3A-C4A	3.14	120.20	111.77
47	S1	607	CHL	C3C-C4C-NC	-3.14	107.06	110.57
31	B	607	CLA	C2C-C1C-NC	3.14	112.91	109.97
47	S	601	CHL	C3C-C4C-NC	-3.13	107.06	110.57
47	n1	606	CHL	C4A-NA-C1A	3.13	108.11	106.71
31	G1	614	CLA	C2C-C1C-NC	3.13	112.91	109.97
47	y1	607	CHL	C2C-C3C-C4C	3.13	108.72	106.49
49	G	622	XAT	C38-C25-C26	-3.13	117.01	122.26
33	c	517	BCR	C3-C4-C5	-3.13	108.48	114.08
47	g1	606	CHL	C3C-C4C-NC	-3.13	107.06	110.57
45	f1	101	HEM	CMC-C2C-C3C	3.13	130.54	124.68
31	S	605	CLA	CHD-C1D-ND	-3.13	121.58	124.45
47	y1	601	CHL	CMA-C3A-C4A	3.13	120.19	111.77
31	N	603	CLA	C1-C2-C3	-3.13	120.62	126.04
31	c1	501	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	A1	405	CLA	CBC-CAC-C3C	3.13	121.06	112.43
31	y1	602	CLA	CHD-C1D-ND	-3.13	121.58	124.45
31	R1	602	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	g1	603	CLA	C2C-C1C-NC	3.13	112.90	109.97
48	G1	620	LUT	C18-C5-C6	-3.13	121.01	124.53
48	Y1	620	LUT	C18-C5-C6	-3.13	121.01	124.53
31	a1	406	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	C1	511	CLA	CHD-C1D-ND	-3.13	121.58	124.45
47	g1	605	CHL	C2C-C3C-C4C	3.13	108.72	106.49
35	d	411	LMG	O8-C28-C29	3.13	121.72	111.91
31	s	610	CLA	CMA-C3A-C4A	3.13	120.18	111.77
31	C	502	CLA	CHD-C1D-ND	-3.13	121.58	124.45
48	S	620	LUT	C38-C25-C24	-3.13	116.87	123.56
31	C1	501	CLA	CMA-C3A-C4A	3.12	120.17	111.77
31	s	613	CLA	CMA-C3A-C4A	3.12	120.17	111.77
47	g1	608	CHL	CMA-C3A-C4A	3.12	120.17	111.77
47	g	605	CHL	C2C-C3C-C4C	3.12	108.72	106.49
31	N	614	CLA	CHD-C1D-ND	-3.12	121.58	124.45
31	R	613	CLA	CHD-C1D-ND	-3.12	121.58	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a1	405	CLA	C2D-C1D-ND	3.12	112.41	110.10
33	c	514	BCR	C31-C1-C6	-3.12	105.23	110.30
37	B	620	C7Z	C2-C3-C4	3.12	114.58	110.30
45	f	101	HEM	C1B-NB-C4B	3.12	108.30	105.07
37	b1	620	C7Z	C2-C3-C4	3.12	114.58	110.30
47	r1	607	CHL	C2C-C3C-C4C	3.12	108.71	106.49
31	N	610	CLA	C2D-C1D-ND	3.12	112.40	110.10
56	r1	626	ERG	C14-C8-C7	-3.12	118.23	124.38
47	Y	609	CHL	C2C-C3C-C4C	3.12	108.71	106.49
31	s	609	CLA	CHD-C1D-ND	-3.12	121.59	124.45
31	n1	603	CLA	CHD-C1D-ND	-3.12	121.59	124.45
47	y1	606	CHL	CMA-C3A-C4A	3.12	120.16	111.77
31	B1	614	CLA	C2C-C1C-NC	3.12	112.89	109.97
31	S1	612	CLA	C2C-C1C-NC	3.12	112.89	109.97
31	a1	406	CLA	C2C-C1C-NC	3.12	112.89	109.97
47	S1	601	CHL	C2C-C3C-C4C	3.12	108.71	106.49
31	B	604	CLA	C1-C2-C3	-3.12	120.65	126.04
31	b	603	CLA	C2D-C1D-ND	3.12	112.40	110.10
31	c	505	CLA	C2C-C1C-NC	3.12	112.89	109.97
31	R1	608	CLA	C2C-C1C-NC	3.12	112.89	109.97
47	s1	608	CHL	C3C-C4C-NC	-3.12	107.08	110.57
47	y1	605	CHL	C3C-C4C-NC	-3.12	107.08	110.57
31	n	603	CLA	C1-C2-C3	-3.12	120.65	126.04
31	c1	509	CLA	C2C-C1C-NC	3.12	112.89	109.97
47	N1	608	CHL	C3C-C4C-NC	-3.12	107.08	110.57
31	a1	410	CLA	CHD-C1D-ND	-3.12	121.59	124.45
48	s	620	LUT	C7-C8-C9	-3.12	121.53	126.23
33	B	619	BCR	C36-C18-C17	-3.11	118.56	122.92
31	B	607	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	g	614	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	s1	604	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	y1	614	CLA	C2C-C1C-NC	3.11	112.89	109.97
31	d	402	CLA	C2D-C1D-ND	3.11	112.40	110.10
31	s	609	CLA	C2C-C1C-NC	3.11	112.89	109.97
31	C1	501	CLA	C2C-C1C-NC	3.11	112.89	109.97
31	D1	403	CLA	C2C-C1C-NC	3.11	112.89	109.97
31	S1	617	CLA	CMA-C3A-C4A	3.11	120.14	111.77
47	s	607	CHL	CMA-C3A-C4A	3.11	120.14	111.77
46	h	101	RRX	C30-C25-C26	-3.11	118.23	122.61
31	C	503	CLA	CMA-C3A-C4A	3.11	120.13	111.77
31	R	613	CLA	C2C-C1C-NC	3.11	112.89	109.97
46	H	101	RRX	C38-C26-C27	3.11	120.12	114.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B1	616	CLA	CHD-C1D-ND	-3.11	121.60	124.45
31	b	608	CLA	C2C-C1C-NC	3.11	112.89	109.97
48	n	620	LUT	C31-C32-C33	-3.11	117.68	126.42
31	c1	511	CLA	CHD-C1D-ND	-3.11	121.60	124.45
31	s	614	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
47	s	608	CHL	CMA-C3A-C4A	3.11	120.13	111.77
31	G	603	CLA	CBC-CAC-C3C	-3.11	103.86	112.43
31	c	507	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
47	g1	608	CHL	CHD-C1D-ND	-3.11	121.60	124.45
31	N	604	CLA	C1-C2-C3	-3.11	120.67	126.04
31	b	615	CLA	C1-C2-C3	-3.11	120.67	126.04
31	b	611	CLA	C1-C2-C3	-3.11	120.67	126.04
33	c	516	BCR	C33-C5-C4	3.11	119.58	113.62
47	S	601	CHL	CMA-C3A-C4A	3.10	120.12	111.77
31	N1	603	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	B	616	CLA	C2D-C1D-ND	3.10	112.39	110.10
47	N1	606	CHL	C2C-C3C-C4C	3.10	108.70	106.49
47	n1	609	CHL	C2C-C3C-C4C	3.10	108.70	106.49
31	g	612	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	c1	503	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	y	602	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
31	C	511	CLA	CMA-C3A-C4A	3.10	120.11	111.77
31	s	617	CLA	CMA-C3A-C4A	3.10	120.11	111.77
31	N	602	CLA	CHD-C1D-ND	-3.10	121.60	124.45
47	n1	608	CHL	CHD-C1D-ND	-3.10	121.60	124.45
31	B1	615	CLA	C1-C2-C3	-3.10	120.68	126.04
31	D	403	CLA	C2D-C1D-ND	3.10	112.39	110.10
31	G1	612	CLA	C2C-C1C-NC	3.10	112.88	109.97
37	B1	620	C7Z	C23-C24-C25	3.10	118.03	111.85
31	B	608	CLA	CHD-C1D-ND	-3.10	121.60	124.45
31	r	613	CLA	CHD-C1D-ND	-3.10	121.60	124.45
37	b1	620	C7Z	C31-C30-C29	-3.10	122.88	127.31
47	G	605	CHL	C3C-C4C-NC	-3.10	107.09	110.57
50	R1	622	NEX	C39-C29-C30	-3.10	118.58	122.92
31	C	508	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	n1	603	CLA	C1-C2-C3	-3.10	120.68	126.04
31	C	503	CLA	C2D-C1D-ND	3.10	112.39	110.10
47	n	601	CHL	C2C-C3C-C4C	3.10	108.70	106.49
47	n1	608	CHL	C3C-C4C-NC	-3.10	107.10	110.57
31	r1	608	CLA	CMA-C3A-C4A	3.10	120.10	111.77
31	s1	605	CLA	CMA-C3A-C4A	3.10	120.10	111.77
40	c1	519	DGD	O1G-C1A-C2A	3.10	121.62	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	R1	607	CHL	CMA-C3A-C4A	3.10	120.09	111.77
47	Y1	609	CHL	C1B-CHB-C4A	-3.10	123.98	130.12
31	c1	508	CLA	C1-C2-C3	-3.10	120.69	126.04
47	n	606	CHL	C2C-C3C-C4C	3.10	108.70	106.49
31	G	603	CLA	C2D-C1D-ND	3.10	112.39	110.10
31	N	614	CLA	CMA-C3A-C4A	3.10	120.09	111.77
31	d1	402	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	c	504	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
48	y	621	LUT	C35-C15-C14	-3.09	117.14	123.47
31	N	603	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	g1	613	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	A1	410	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	a1	407	CLA	C2D-C1D-ND	3.09	112.38	110.10
31	S	610	CLA	C2C-C1C-NC	3.09	112.87	109.97
47	r	606	CHL	CMA-C3A-C4A	3.09	120.08	111.77
31	C1	505	CLA	C1-C2-C3	-3.09	120.69	126.04
31	c	503	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	R1	609	CLA	C2C-C1C-NC	3.09	112.87	109.97
32	A	408	PHO	CMB-C2B-C3B	3.09	130.46	124.68
31	R1	609	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	y1	613	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	b	602	CLA	C2C-C1C-NC	3.09	112.87	109.97
48	S1	620	LUT	C11-C10-C9	-3.09	122.90	127.31
47	g1	605	CHL	CMA-C3A-C4A	3.09	120.08	111.77
31	B	615	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	B	609	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
47	S	606	CHL	C3C-C4C-NC	-3.09	107.11	110.57
31	c1	509	CLA	CMA-C3A-C4A	3.09	120.07	111.77
31	A1	410	CLA	C2C-C1C-NC	3.09	112.86	109.97
48	Y1	621	LUT	C18-C5-C6	-3.09	121.06	124.53
31	g	610	CLA	CMA-C3A-C4A	3.09	120.07	111.77
31	R	604	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	g	603	CLA	CHD-C1D-ND	-3.08	121.62	124.45
32	a1	408	PHO	O1D-CGD-CBD	3.08	129.88	124.74
31	b	605	CLA	CMA-C3A-C4A	3.08	120.06	111.77
31	b	615	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
47	y	605	CHL	C3C-C4C-NC	-3.08	107.11	110.57
31	B1	610	CLA	CMB-C2B-C3B	3.08	130.44	124.68
31	R	608	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	Y	612	CLA	C2C-C1C-NC	3.08	112.86	109.97
49	g	622	XAT	O24-C25-C24	3.08	115.70	113.38
31	R1	604	CLA	CHD-C1D-ND	-3.08	121.62	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	611	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	R1	609	CLA	CMA-C3A-C4A	3.08	120.05	111.77
47	n	608	CHL	CHB-C4A-NA	3.08	128.77	124.51
31	S	604	CLA	C2C-C1C-NC	3.08	112.86	109.97
49	r	622	XAT	O4-C5-C4	-3.08	111.07	113.38
31	b1	613	CLA	CMA-C3A-C4A	3.08	120.05	111.77
31	s	602	CLA	C2D-C1D-ND	3.08	112.37	110.10
47	r1	607	CHL	C3C-C4C-NC	-3.08	107.12	110.57
31	s	611	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	s1	609	CLA	C1-C2-C3	-3.08	120.72	126.04
31	b	610	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	s1	617	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	A	410	CLA	CHD-C1D-ND	-3.08	121.62	124.45
47	n1	606	CHL	C2C-C3C-C4C	3.08	108.68	106.49
31	y	610	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	y1	610	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	Y	603	CLA	C2C-C1C-NC	3.08	112.85	109.97
31	g1	611	CLA	C2C-C1C-NC	3.08	112.85	109.97
31	n1	611	CLA	CHD-C1D-ND	-3.08	121.63	124.45
33	b1	619	BCR	C33-C5-C6	-3.08	121.07	124.53
31	C1	504	CLA	C1-C2-C3	-3.08	120.72	126.04
31	S1	604	CLA	CHD-C1D-ND	-3.08	121.63	124.45
32	a	408	PHO	CMB-C2B-C3B	3.07	130.43	124.68
40	c1	520	DGD	O6D-C5D-C6D	3.07	112.87	106.67
31	Y	614	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	C1	513	CLA	CHD-C1D-ND	-3.07	121.63	124.45
47	N	606	CHL	C2C-C3C-C4C	3.07	108.68	106.49
33	b	619	BCR	C37-C22-C21	-3.07	118.62	122.92
47	g	608	CHL	C3C-C4C-NC	-3.07	107.13	110.57
47	g1	607	CHL	CMA-C3A-C4A	3.07	120.03	111.77
31	B1	614	CLA	C2D-C1D-ND	3.07	112.37	110.10
31	G1	612	CLA	C2D-C1D-ND	3.07	112.37	110.10
31	R	608	CLA	C1-C2-C3	-3.07	120.73	126.04
47	N	609	CHL	C3C-C4C-NC	-3.07	107.13	110.57
31	N1	604	CLA	C2C-C1C-NC	3.07	112.85	109.97
48	g1	620	LUT	C18-C5-C6	-3.07	121.08	124.53
31	B	610	CLA	C2D-C1D-ND	3.07	112.37	110.10
49	N1	622	XAT	C38-C25-C26	-3.07	117.12	122.26
47	g1	605	CHL	C3C-C4C-NC	-3.07	107.13	110.57
31	y1	602	CLA	C2D-C1D-ND	3.07	112.36	110.10
31	y	602	CLA	CHD-C1D-ND	-3.07	121.64	124.45
31	D1	403	CLA	CHD-C1D-ND	-3.07	121.64	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	n	607	CHL	C3C-C4C-NC	-3.07	107.13	110.57
47	y	607	CHL	CHB-C4A-NA	3.07	128.75	124.51
47	G1	605	CHL	C2C-C3C-C4C	3.07	108.67	106.49
47	s1	606	CHL	C2C-C3C-C4C	3.07	108.67	106.49
47	s1	606	CHL	C3C-C4C-NC	-3.07	107.13	110.57
31	N1	602	CLA	CHD-C1D-ND	-3.07	121.64	124.45
50	S1	623	NEX	C39-C29-C30	-3.07	118.63	122.92
47	g	601	CHL	CMA-C3A-C4A	3.07	120.01	111.77
31	s1	612	CLA	CMB-C2B-C3B	3.07	130.41	124.68
31	a1	410	CLA	C2C-C1C-NC	3.07	112.84	109.97
47	N	607	CHL	CHD-C1D-ND	-3.07	121.64	124.45
31	s1	611	CLA	CMA-C3A-C4A	3.07	120.01	111.77
47	R	607	CHL	C3C-C4C-NC	-3.06	107.13	110.57
31	B1	603	CLA	C1-C2-C3	-3.06	120.74	126.04
33	c1	517	BCR	C33-C5-C4	3.06	119.50	113.62
31	B1	606	CLA	C1-C2-C3	-3.06	120.75	126.04
31	n1	614	CLA	CMA-C3A-C4A	3.06	120.01	111.77
31	g	602	CLA	CMA-C3A-C4A	3.06	120.00	111.77
50	g	623	NEX	C39-C29-C30	-3.06	118.63	122.92
48	n1	621	LUT	C18-C5-C6	-3.06	121.09	124.53
31	Y	611	CLA	C2C-C1C-NC	3.06	112.84	109.97
31	n	614	CLA	C2D-C1D-ND	3.06	112.36	110.10
47	N1	609	CHL	CHB-C4A-NA	3.06	128.75	124.51
31	g	612	CLA	CHD-C1D-ND	-3.06	121.64	124.45
47	n	607	CHL	C1-C2-C3	-3.06	120.75	126.04
47	s1	608	CHL	CMA-C3A-C4A	3.06	120.00	111.77
31	Y1	603	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
47	y	607	CHL	C3C-C4C-NC	-3.06	107.14	110.57
31	N1	603	CLA	C1-C2-C3	-3.06	120.75	126.04
48	n1	621	LUT	C15-C14-C13	-3.06	122.94	127.31
47	s1	607	CHL	C3C-C4C-NC	-3.06	107.14	110.57
47	g	601	CHL	C1-O2A-CGA	3.06	124.47	116.44
31	s	617	CLA	C2D-C1D-ND	3.06	112.36	110.10
31	A1	406	CLA	C2D-C1D-ND	3.06	112.36	110.10
31	B1	611	CLA	CHD-C1D-ND	-3.06	121.64	124.45
45	f1	101	HEM	C4D-ND-C1D	3.06	108.23	105.07
31	Y	603	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
33	c	515	BCR	C33-C5-C6	-3.06	121.10	124.53
47	S	606	CHL	CMA-C3A-C4A	3.06	119.99	111.77
31	C1	508	CLA	CMB-C2B-C3B	3.06	130.40	124.68
47	y	605	CHL	CMA-C3A-C4A	3.06	119.98	111.77
47	Y1	607	CHL	CHB-C4A-NA	3.06	128.74	124.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B1	613	CLA	CMA-C3A-C4A	3.05	119.98	111.77
31	B1	607	CLA	CMB-C2B-C3B	3.05	130.39	124.68
31	Y1	604	CLA	C2D-C1D-ND	3.05	112.36	110.10
32	a	409	PHO	O1D-CGD-CBD	3.05	129.83	124.74
47	Y	609	CHL	C1-O2A-CGA	3.05	124.46	116.44
47	g	608	CHL	C2C-C3C-C4C	3.05	108.67	106.49
31	b1	617	CLA	C1-C2-C3	-3.05	120.76	126.04
31	g	604	CLA	C2C-C1C-NC	3.05	112.83	109.97
31	s	604	CLA	C2C-C1C-NC	3.05	112.83	109.97
31	r1	602	CLA	C2D-C1D-ND	3.05	112.35	110.10
48	y	621	LUT	C38-C25-C24	-3.05	117.03	123.56
33	c	516	BCR	C37-C22-C23	3.05	122.88	118.08
31	B1	603	CLA	C2D-C1D-ND	3.05	112.35	110.10
31	c	508	CLA	CMB-C2B-C3B	3.05	130.38	124.68
47	N	607	CHL	CMA-C3A-C4A	3.05	119.97	111.77
31	b1	606	CLA	CHD-C1D-ND	-3.05	121.65	124.45
48	G	621	LUT	C11-C10-C9	-3.05	122.96	127.31
47	N	601	CHL	CMA-C3A-C4A	3.05	119.97	111.77
33	C1	516	BCR	C36-C18-C17	-3.05	118.65	122.92
31	R	602	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	r	609	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	b1	614	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	N1	614	CLA	C2C-C1C-NC	3.05	112.83	109.97
37	b	620	C7Z	C1-C6-C5	-3.05	118.32	122.61
31	C1	510	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
31	s1	604	CLA	CMA-C3A-C4A	3.04	119.96	111.77
33	d	404	BCR	C38-C26-C27	3.04	119.47	113.62
31	G	611	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	s1	613	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	a	407	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	c1	507	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	C1	506	CLA	C2C-C1C-NC	3.04	112.82	109.97
47	G	605	CHL	CMA-C3A-C4A	3.04	119.95	111.77
49	R1	621	XAT	O24-C25-C24	3.04	115.67	113.38
31	S1	612	CLA	C2D-C1D-ND	3.04	112.35	110.10
31	b1	609	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
44	D1	405	PL9	C7-C8-C9	-3.04	121.73	126.79
31	G	611	CLA	C2D-C1D-ND	3.04	112.34	110.10
31	n1	613	CLA	CBA-CAA-C2A	3.04	122.83	113.86
31	c	510	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
31	n1	611	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	a1	406	CLA	C1-C2-C3	-3.04	120.79	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	G1	607	CHL	CHD-C1D-ND	-3.04	121.66	124.45
49	n1	622	XAT	C6-C7-C8	-3.04	119.57	125.99
47	G	609	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
31	C	510	CLA	CHD-C1D-ND	-3.04	121.66	124.45
47	G1	609	CHL	CMA-C3A-C4A	3.03	119.93	111.77
31	b	603	CLA	C2C-C1C-NC	3.03	112.81	109.97
47	N	609	CHL	CMA-C3A-C4A	3.03	119.93	111.77
31	S1	602	CLA	CHD-C1D-ND	-3.03	121.67	124.45
31	D	403	CLA	C2C-C1C-NC	3.03	112.81	109.97
48	g	620	LUT	C18-C5-C6	-3.03	121.12	124.53
56	r1	626	ERG	C1-C2-C3	3.03	114.36	110.47
31	R1	603	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	g1	604	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	y1	612	CLA	C1-C2-C3	-3.03	120.80	126.04
31	r1	609	CLA	CMA-C3A-C4A	3.03	119.92	111.77
31	y1	602	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
31	c1	508	CLA	CMB-C2B-C3B	3.03	130.35	124.68
31	b	615	CLA	CBA-CAA-C2A	3.03	122.81	113.86
31	c	511	CLA	CHD-C1D-ND	-3.03	121.67	124.45
31	d1	402	CLA	CHD-C1D-ND	-3.03	121.67	124.45
47	N	608	CHL	C3C-C4C-NC	-3.03	107.17	110.57
47	Y1	606	CHL	C3C-C4C-NC	-3.03	107.17	110.57
31	Y1	611	CLA	C1-C2-C3	-3.03	120.80	126.04
31	Y	610	CLA	CHD-C1D-ND	-3.03	121.67	124.45
31	G	610	CLA	C1-C2-C3	-3.03	120.80	126.04
31	C	512	CLA	C2C-C1C-NC	3.03	112.81	109.97
47	n1	607	CHL	CMA-C3A-C4A	3.03	119.91	111.77
47	Y	607	CHL	C3C-C4C-NC	-3.03	107.17	110.57
31	S	609	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	c1	513	CLA	C2D-C1D-ND	3.03	112.33	110.10
33	c1	515	BCR	C31-C1-C6	-3.03	105.39	110.30
31	B1	606	CLA	CMD-C2D-C3D	-3.03	120.65	127.61
31	a	406	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	N	602	CLA	CMA-C3A-C4A	3.03	119.91	111.77
47	r1	606	CHL	CMA-C3A-C4A	3.03	119.91	111.77
54	I1	102	4RF	O40-C41-C43	3.03	121.40	111.91
31	c1	504	CLA	C2D-C1D-ND	3.02	112.33	110.10
31	B1	612	CLA	CMC-C2C-C1C	3.02	129.65	125.04
35	a	413	LMG	O8-C28-C29	3.02	121.40	111.91
31	n1	602	CLA	C2C-C1C-NC	3.02	112.81	109.97
47	y	609	CHL	C3C-C4C-NC	-3.02	107.18	110.57
48	Y1	620	LUT	C11-C10-C9	-3.02	123.00	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	613	CLA	CMB-C2B-C3B	3.02	130.33	124.68
33	c	515	BCR	C1-C6-C5	-3.02	118.36	122.61
31	c1	509	CLA	CHD-C1D-ND	-3.02	121.68	124.45
31	r1	610	CLA	CHD-C1D-ND	-3.02	121.68	124.45
31	g1	603	CLA	CMA-C3A-C4A	3.02	119.89	111.77
47	g	605	CHL	CMA-C3A-C4A	3.02	119.89	111.77
31	N	611	CLA	CMA-C3A-C4A	3.02	119.89	111.77
32	a	409	PHO	O2D-CGD-O1D	-3.02	117.93	123.84
50	g1	623	NEX	C16-C1-C6	-3.02	107.77	110.47
31	n	610	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	S1	609	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	n	603	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
50	N1	623	NEX	C17-C1-C6	-3.02	107.77	110.47
31	A	407	CLA	CMA-C3A-C4A	3.02	119.88	111.77
31	G	614	CLA	CMA-C3A-C4A	3.02	119.88	111.77
31	y	608	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	C	507	CLA	CHD-C1D-ND	-3.02	121.68	124.45
31	n1	610	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	b	614	CLA	C2D-C1D-ND	3.02	112.33	110.10
47	s	601	CHL	C3C-C4C-NC	-3.02	107.19	110.57
31	b1	615	CLA	C1-C2-C3	-3.02	120.83	126.04
31	c	504	CLA	CMB-C2B-C3B	3.02	130.32	124.68
33	c	516	BCR	C19-C18-C17	3.02	123.57	118.94
31	B	614	CLA	CHD-C1D-ND	-3.02	121.68	124.45
47	y1	607	CHL	C3C-C4C-NC	-3.01	107.19	110.57
31	N	613	CLA	CHD-C1D-ND	-3.01	121.68	124.45
31	G	604	CLA	CHD-C1D-ND	-3.01	121.68	124.45
47	y	609	CHL	CMA-C3A-C4A	3.01	119.87	111.77
31	S1	602	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
31	r	602	CLA	C2C-C1C-NC	3.01	112.80	109.97
31	n1	604	CLA	CHD-C1D-ND	-3.01	121.69	124.45
49	r	622	XAT	O24-C25-C24	3.01	115.64	113.38
31	C	513	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	c1	502	CLA	C1-C2-C3	-3.01	120.83	126.04
31	c1	502	CLA	CMA-C3A-C4A	3.01	119.87	111.77
31	C	513	CLA	C2D-C1D-ND	3.01	112.32	110.10
47	s	606	CHL	CMA-C3A-C4A	3.01	119.86	111.77
31	C	502	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
48	n1	620	LUT	C15-C14-C13	-3.01	123.01	127.31
31	R	609	CLA	C1-C2-C3	-3.01	120.84	126.04
31	B1	610	CLA	C2D-C1D-ND	3.01	112.32	110.10
31	g1	602	CLA	C2D-C1D-ND	3.01	112.32	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g1	606	CHL	CMA-C3A-C4A	3.01	119.86	111.77
47	s	607	CHL	C2C-C3C-C4C	3.01	108.63	106.49
31	g1	613	CLA	CMA-C3A-C4A	3.01	119.86	111.77
47	N	608	CHL	C1-O2A-CGA	3.01	124.34	116.44
31	c1	508	CLA	CHD-C1D-ND	-3.01	121.69	124.45
31	A	410	CLA	CMA-C3A-C4A	3.01	119.86	111.77
47	Y1	609	CHL	CMA-C3A-C4A	3.01	119.86	111.77
40	b1	623	DGD	O1G-C1A-C2A	3.01	121.35	111.91
31	c	508	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
31	G1	611	CLA	CMA-C3A-C4A	3.01	119.86	111.77
47	S1	606	CHL	C2C-C3C-C4C	3.01	108.63	106.49
31	n1	613	CLA	C2D-C1D-ND	3.01	112.32	110.10
31	B1	611	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
47	s	607	CHL	C3C-C4C-NC	-3.01	107.20	110.57
47	S1	606	CHL	C3C-C4C-NC	-3.01	107.20	110.57
31	b	611	CLA	CHD-C1D-ND	-3.01	121.69	124.45
31	B1	602	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
31	b1	603	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
31	y	611	CLA	CHD-C1D-ND	-3.00	121.69	124.45
48	S	621	LUT	C31-C30-C29	-3.00	123.02	127.31
31	C	502	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	N	604	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	G1	614	CLA	C2D-C1D-ND	3.00	112.32	110.10
48	s	620	LUT	C38-C25-C24	-3.00	117.14	123.56
31	R	608	CLA	CHD-C1D-ND	-3.00	121.69	124.45
47	N1	606	CHL	CHB-C4A-NA	3.00	128.66	124.51
31	Y	608	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	A1	407	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	B1	609	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
33	D1	404	BCR	C34-C9-C10	-3.00	118.72	122.92
48	G	621	LUT	C10-C11-C12	-3.00	113.85	123.22
31	g1	613	CLA	C2C-C1C-NC	3.00	112.78	109.97
46	H1	101	RRX	C36-C18-C19	3.00	122.80	118.08
31	c1	504	CLA	C1-C2-C3	-3.00	120.86	126.04
31	y1	608	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	R1	608	CLA	CMA-C3A-C4A	3.00	119.83	111.77
31	Y	610	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	g1	613	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	b1	608	CLA	CMB-C2B-C3B	3.00	130.29	124.68
49	R	621	XAT	C18-C5-C6	-3.00	117.24	122.26
47	N1	608	CHL	C2C-C3C-C4C	3.00	108.63	106.49
31	Y1	610	CLA	CHD-C1D-ND	-3.00	121.70	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	609	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
31	r	603	CLA	CHD-C1D-ND	-3.00	121.70	124.45
31	s	612	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	n1	613	CLA	C2C-C1C-NC	3.00	112.78	109.97
32	A1	408	PHO	CMB-C2B-C3B	3.00	130.28	124.68
33	c	515	BCR	C8-C7-C6	-3.00	118.79	127.20
31	Y	614	CLA	C1-C2-C3	-3.00	120.86	126.04
31	Y1	614	CLA	C1-C2-C3	-3.00	120.86	126.04
31	R1	609	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	d	403	CLA	CMA-C3A-C4A	3.00	119.82	111.77
31	b1	612	CLA	CMA-C3A-C4A	3.00	119.82	111.77
31	b1	612	CLA	C1-C2-C3	-3.00	120.86	126.04
31	a1	407	CLA	CMA-C3A-C4A	2.99	119.82	111.77
31	C	510	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
50	g	623	NEX	C17-C1-C6	-2.99	107.79	110.47
47	Y1	609	CHL	C4D-CHA-C1A	2.99	124.89	121.25
31	a	405	CLA	CMB-C2B-C3B	2.99	130.28	124.68
47	s1	606	CHL	CMA-C3A-C4A	2.99	119.82	111.77
47	S1	607	CHL	CMA-C3A-C4A	2.99	119.81	111.77
31	C	501	CLA	CMD-C2D-C3D	-2.99	120.73	127.61
31	B	609	CLA	C1-C2-C3	-2.99	120.87	126.04
31	s	603	CLA	CHD-C1D-ND	-2.99	121.70	124.45
31	G1	603	CLA	CHD-C1D-ND	-2.99	121.70	124.45
47	G1	605	CHL	C3C-C4C-NC	-2.99	107.22	110.57
31	Y	608	CLA	CMA-C3A-C4A	2.99	119.81	111.77
44	D	405	PL9	C40-C39-C41	2.99	120.30	115.27
33	B	619	BCR	C19-C18-C17	2.99	123.53	118.94
47	Y1	605	CHL	C3C-C4C-NC	-2.99	107.22	110.57
31	C	511	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	B1	605	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	G1	613	CLA	C2C-C1C-NC	2.99	112.77	109.97
47	S1	608	CHL	C1-O2A-CGA	2.99	124.28	116.44
31	N1	604	CLA	CHD-C1D-ND	-2.99	121.71	124.45
47	g1	601	CHL	C2C-C3C-C4C	2.99	108.62	106.49
48	G	620	LUT	C22-C23-C24	-2.99	108.34	111.74
47	n1	608	CHL	CMA-C3A-C4A	2.99	119.80	111.77
31	n	611	CLA	CHD-C1D-ND	-2.99	121.71	124.45
50	N1	623	NEX	C38-C25-C26	-2.99	117.26	122.26
31	B	609	CLA	CMA-C3A-C4A	2.99	119.80	111.77
47	s	601	CHL	C2C-C3C-C4C	2.99	108.62	106.49
50	Y	623	NEX	C16-C1-C6	-2.98	107.80	110.47
31	g	614	CLA	CMA-C3A-C4A	2.98	119.79	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g1	620	LUT	C31-C30-C29	-2.98	123.05	127.31
47	N1	607	CHL	C2C-C3C-C4C	2.98	108.62	106.49
33	b1	619	BCR	C4-C5-C6	-2.98	118.40	122.73
31	C	504	CLA	C2C-C1C-NC	2.98	112.77	109.97
31	R1	602	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
31	b	603	CLA	CMA-C3A-C4A	2.98	119.79	111.77
31	b	614	CLA	C2C-C1C-NC	2.98	112.77	109.97
46	h	101	RRX	C33-C5-C6	-2.98	121.18	124.53
31	c	513	CLA	C1-C2-C3	-2.98	120.89	126.04
31	R	610	CLA	C2C-C1C-NC	2.98	112.77	109.97
47	s1	608	CHL	C2C-C3C-C4C	2.98	108.61	106.49
47	Y	607	CHL	C1-O2A-CGA	2.98	124.26	116.44
31	c1	508	CLA	C1D-ND-C4D	-2.98	104.22	106.33
47	r	607	CHL	CMA-C3A-C4A	2.98	119.78	111.77
33	c1	517	BCR	C36-C18-C17	-2.98	118.75	122.92
31	r1	608	CLA	C1-C2-C3	-2.98	120.89	126.04
31	s1	610	CLA	CHD-C1D-ND	-2.98	121.72	124.45
31	a1	406	CLA	CMA-C3A-C4A	2.98	119.77	111.77
31	Y1	608	CLA	CHD-C1D-ND	-2.98	121.72	124.45
31	G1	604	CLA	C2C-C1C-NC	2.98	112.76	109.97
31	c	513	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	Y	604	CLA	C1-C2-C3	-2.98	120.90	126.04
31	B1	612	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
31	R	602	CLA	C1-C2-C3	-2.97	120.90	126.04
31	r	602	CLA	C1-C2-C3	-2.97	120.90	126.04
31	s	605	CLA	CMA-C3A-C4A	2.97	119.77	111.77
31	d	403	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
31	y1	604	CLA	C1-C2-C3	-2.97	120.90	126.04
31	B1	605	CLA	CHD-C1D-ND	-2.97	121.72	124.45
47	s	606	CHL	C3C-C4C-NC	-2.97	107.24	110.57
47	G1	608	CHL	C2C-C3C-C4C	2.97	108.61	106.49
50	N	623	NEX	C39-C29-C30	-2.97	118.76	122.92
35	a	413	LMG	C8-O7-C10	-2.97	110.47	117.79
31	y1	603	CLA	C2D-C1D-ND	2.97	112.29	110.10
49	Y1	622	XAT	C38-C25-C26	-2.97	117.28	122.26
47	G1	608	CHL	C3C-C4C-NC	-2.97	107.24	110.57
47	Y1	609	CHL	C3C-C4C-NC	-2.97	107.24	110.57
33	C1	516	BCR	C28-C27-C26	-2.97	108.77	114.08
50	Y1	623	NEX	C39-C29-C30	-2.97	118.76	122.92
31	D	402	CLA	C1-C2-C3	-2.97	120.91	126.04
31	N1	614	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	r	611	CLA	CMA-C3A-C4A	2.97	119.75	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	608	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	b	617	CLA	C2C-C1C-NC	2.97	112.75	109.97
31	B1	610	CLA	CHD-C1D-ND	-2.97	121.73	124.45
31	y	610	CLA	C1-C2-C3	-2.97	120.91	126.04
31	c	502	CLA	CMA-C3A-C4A	2.97	119.75	111.77
47	Y	605	CHL	CMA-C3A-C4A	2.97	119.75	111.77
31	C	501	CLA	C1-C2-C3	-2.97	120.91	126.04
31	B1	613	CLA	C2C-C1C-NC	2.97	112.75	109.97
31	c1	502	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	N	603	CLA	C1C-C2C-C3C	-2.97	103.84	106.96
48	n	620	LUT	C3-C4-C5	-2.97	105.95	111.85
31	N	602	CLA	C2D-C1D-ND	2.96	112.29	110.10
47	n	609	CHL	C1B-CHB-C4A	-2.96	124.25	130.12
31	y	614	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
49	G1	622	XAT	C19-C9-C10	-2.96	118.77	122.92
31	A1	410	CLA	CMB-C2B-C3B	2.96	130.22	124.68
50	y	623	NEX	C38-C25-C26	-2.96	117.29	122.26
31	D	403	CLA	CMA-C3A-C4A	2.96	119.73	111.77
31	A	405	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
31	Y	608	CLA	C1-C2-C3	-2.96	121.96	126.75
31	N1	603	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
31	r	604	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	r	611	CLA	CHD-C1D-ND	-2.96	121.73	124.45
31	b	612	CLA	CMA-C3A-C4A	2.96	119.73	111.77
31	B1	607	CLA	C2C-C1C-NC	2.96	112.75	109.97
47	G1	609	CHL	C1-O2A-CGA	2.96	124.21	116.44
48	n1	620	LUT	C35-C34-C33	-2.96	123.09	127.31
31	r1	610	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	C1	508	CLA	CMA-C3A-C4A	2.96	119.73	111.77
47	y1	609	CHL	CMA-C3A-C4A	2.96	119.73	111.77
47	s1	601	CHL	CMA-C3A-C4A	2.96	119.73	111.77
31	b1	605	CLA	CHD-C1D-ND	-2.96	121.73	124.45
47	G	601	CHL	CMA-C3A-C4A	2.96	119.72	111.77
47	n1	605	CHL	CMA-C3A-C4A	2.96	119.72	111.77
31	Y	611	CLA	CMA-C3A-C4A	2.96	119.72	111.77
31	g1	610	CLA	C2C-C1C-NC	2.96	112.74	109.97
47	y	606	CHL	C2C-C3C-C4C	2.96	108.60	106.49
47	g	606	CHL	C1-O2A-CGA	2.96	124.20	116.44
31	c1	506	CLA	CHD-C1D-ND	-2.96	121.74	124.45
48	N1	620	LUT	C38-C25-C24	-2.96	117.24	123.56
47	S1	601	CHL	C3C-C4C-NC	-2.95	107.26	110.57
31	S1	603	CLA	C1-C2-C3	-2.95	120.93	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B1	602	CLA	CHD-C1D-ND	-2.95	121.74	124.45
31	n1	603	CLA	CMA-C3A-C4A	2.95	119.71	111.77
31	B	604	CLA	C2C-C1C-NC	2.95	112.74	109.97
33	A1	411	BCR	C15-C14-C13	-2.95	123.09	127.31
48	S	621	LUT	C15-C14-C13	-2.95	123.09	127.31
47	S	607	CHL	C3C-C4C-NC	-2.95	107.26	110.57
47	y	606	CHL	C3C-C4C-NC	-2.95	107.26	110.57
31	c	504	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
31	N1	602	CLA	C1-C2-C3	-2.95	120.94	126.04
31	c1	512	CLA	C1-C2-C3	-2.95	120.94	126.04
31	R	611	CLA	C2D-C1D-ND	2.95	112.28	110.10
48	s	621	LUT	C11-C10-C9	-2.95	123.10	127.31
31	N	602	CLA	C1-C2-C3	-2.95	120.94	126.04
31	b1	602	CLA	CHD-C1D-ND	-2.95	121.74	124.45
31	G1	602	CLA	CMC-C2C-C1C	2.95	129.53	125.04
33	a1	411	BCR	C15-C14-C13	-2.95	123.10	127.31
31	S1	609	CLA	C2D-C1D-ND	2.95	112.28	110.10
31	B	602	CLA	CHD-C1D-ND	-2.95	121.74	124.45
31	r1	612	CLA	CHD-C1D-ND	-2.95	121.74	124.45
31	y1	614	CLA	CMD-C2D-C3D	-2.95	120.83	127.61
31	R1	604	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
31	n	613	CLA	CAC-C3C-C4C	2.95	128.64	124.81
31	C1	503	CLA	CMA-C3A-C4A	2.95	119.70	111.77
50	s	623	NEX	C27-C28-C29	-2.95	120.95	125.53
31	y	614	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	C1	501	CLA	CHD-C1D-ND	-2.95	121.74	124.45
31	n1	614	CLA	C2C-C1C-NC	2.95	112.73	109.97
31	A	406	CLA	CMB-C2B-C3B	2.95	130.19	124.68
31	c1	506	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
31	c	512	CLA	C2D-C1D-ND	2.95	112.28	110.10
48	g	621	LUT	C31-C30-C29	-2.95	123.10	127.31
47	N	605	CHL	C3C-C4C-NC	-2.95	107.27	110.57
31	c1	502	CLA	CHD-C1D-ND	-2.95	121.75	124.45
48	G	621	LUT	C15-C35-C34	-2.95	117.44	123.47
31	y1	603	CLA	C1-C2-C3	-2.95	120.95	126.04
31	R	602	CLA	C2C-C1C-NC	2.95	112.73	109.97
47	g1	601	CHL	C3C-C4C-NC	-2.95	107.27	110.57
47	Y1	601	CHL	CMA-C3A-C4A	2.95	119.69	111.77
31	n	604	CLA	C2D-C1D-ND	2.95	112.28	110.10
31	c1	504	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
31	s	602	CLA	C1-C2-C3	-2.95	120.95	126.04
31	C1	502	CLA	CMA-C3A-C4A	2.95	119.69	111.77

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	501	CLA	C2C-C1C-NC	2.95	112.73	109.97
48	R1	620	LUT	C18-C5-C4	2.94	119.81	114.36
31	S1	609	CLA	CMA-C3A-C4A	2.94	119.69	111.77
50	y1	623	NEX	C1-C2-C3	2.94	120.29	113.64
31	n1	604	CLA	C2D-C1D-ND	2.94	112.27	110.10
31	c	509	CLA	CHD-C1D-ND	-2.94	121.75	124.45
47	n	608	CHL	CHD-C1D-ND	-2.94	121.75	124.45
47	N1	607	CHL	CMA-C3A-C4A	2.94	119.69	111.77
47	S1	608	CHL	CMA-C3A-C4A	2.94	119.69	111.77
31	S1	603	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	r1	602	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	B1	603	CLA	CMA-C3A-C4A	2.94	119.68	111.77
47	s	601	CHL	CMA-C3A-C4A	2.94	119.68	111.77
31	b	617	CLA	C2D-C1D-ND	2.94	112.27	110.10
41	d1	409	LHG	O8-C23-C24	2.94	121.14	111.91
49	r	622	XAT	C31-C30-C29	-2.94	123.11	127.31
31	b	610	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	b1	616	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	A	407	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
31	C	507	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
31	G	602	CLA	C2D-C1D-ND	2.94	112.27	110.10
31	R	611	CLA	CMA-C3A-C4A	2.94	119.68	111.77
49	r	622	XAT	C27-C28-C29	2.94	130.09	125.53
31	n1	613	CLA	C1-C2-C3	-2.94	120.96	126.04
46	H1	101	RRX	C33-C5-C4	2.94	119.27	113.62
31	C1	508	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	C	510	CLA	C1-C2-C3	-2.94	120.96	126.04
31	Y1	613	CLA	CMD-C2D-C3D	-2.94	120.85	127.61
31	g	612	CLA	CMA-C3A-C4A	2.94	119.67	111.77
31	y1	613	CLA	C2C-C1C-NC	2.94	112.72	109.97
33	c	517	BCR	C36-C18-C17	-2.94	118.81	122.92
31	S1	602	CLA	O2A-CGA-CBA	2.94	121.13	111.91
31	g1	604	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	B	604	CLA	CMA-C3A-C4A	2.94	119.67	111.77
31	y1	611	CLA	OBD-CAD-C3D	-2.94	121.45	128.52
31	C	508	CLA	CHD-C1D-ND	-2.94	121.75	124.45
49	N1	622	XAT	O24-C25-C24	2.94	115.59	113.38
31	Y	613	CLA	C2D-C1D-ND	2.94	112.27	110.10
31	S	602	CLA	C1-C2-C3	-2.94	120.97	126.04
31	G	611	CLA	C2C-C1C-NC	2.94	112.72	109.97
31	c1	511	CLA	CAA-C2A-C1A	2.94	121.59	111.97
47	N	601	CHL	C1-O2A-CGA	2.94	124.14	116.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	619	BCR	C33-C5-C6	-2.94	121.23	124.53
31	B1	608	CLA	CMA-C3A-C4A	2.93	119.66	111.77
56	R1	626	ERG	C13-C17-C20	-2.93	115.64	119.43
49	G	622	XAT	C26-C27-C28	-2.93	119.79	125.99
31	b1	608	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	b1	615	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	c1	513	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	b1	607	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	S1	617	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	C	502	CLA	C2C-C1C-NC	2.93	112.72	109.97
31	C1	504	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	C1	512	CLA	CMB-C2B-C3B	2.93	130.16	124.68
44	d	405	PL9	C7-C8-C9	-2.93	121.92	126.79
31	S	605	CLA	CMA-C3A-C4A	2.93	119.64	111.77
48	G1	621	LUT	C31-C32-C33	-2.93	118.19	126.42
31	C1	504	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
31	b	602	CLA	C1-C2-C3	-2.93	120.98	126.04
31	g	611	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	N1	602	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	g	611	CLA	OBD-CAD-C3D	-2.92	121.48	128.52
31	C1	503	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	c1	510	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	y1	612	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	S1	605	CLA	CMA-C3A-C4A	2.92	119.63	111.77
56	r1	626	ERG	C4-C5-C10	2.92	120.31	116.42
47	n1	607	CHL	CHB-C4A-NA	2.92	128.56	124.51
47	Y	609	CHL	CMA-C3A-C4A	2.92	119.63	111.77
47	y	607	CHL	CMA-C3A-C4A	2.92	119.63	111.77
37	b1	620	C7Z	C11-C12-C13	-2.92	118.20	126.42
31	N1	602	CLA	C1D-ND-C4D	-2.92	104.26	106.33
38	j1	101	DGA	OG1-CA1-CA2	2.92	121.08	111.91
33	a	411	BCR	C33-C5-C4	2.92	119.23	113.62
31	B	607	CLA	O2A-CGA-CBA	2.92	121.08	111.91
33	D1	404	BCR	C15-C14-C13	-2.92	123.14	127.31
31	B	615	CLA	C1-C2-C3	-2.92	120.99	126.04
31	B	608	CLA	C2C-C1C-NC	2.92	112.71	109.97
31	G	614	CLA	C2C-C1C-NC	2.92	112.71	109.97
50	Y1	623	NEX	C5-C4-C3	2.92	115.20	111.75
31	S1	604	CLA	CMA-C3A-C4A	2.92	119.62	111.77
31	r	608	CLA	CMD-C2D-C3D	-2.92	120.90	127.61
31	G1	612	CLA	CMA-C3A-C4A	2.92	119.62	111.77
31	B1	604	CLA	C2D-C1D-ND	2.92	112.25	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	610	CLA	O2A-CGA-CBA	2.92	121.07	111.91
50	s	623	NEX	C26-C27-C28	-2.92	119.82	125.99
31	C1	505	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	S	605	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
48	g	621	LUT	C22-C23-C24	-2.92	108.42	111.74
31	b1	604	CLA	CMA-C3A-C4A	2.92	119.61	111.77
48	s1	620	LUT	C35-C34-C33	-2.92	123.15	127.31
33	C1	514	BCR	C33-C5-C6	-2.92	121.25	124.53
31	r	612	CLA	C2C-C1C-NC	2.92	112.70	109.97
33	C1	515	BCR	C34-C9-C10	-2.92	118.84	122.92
49	G1	622	XAT	C26-C27-C28	-2.92	119.83	125.99
47	S1	601	CHL	CMA-C3A-C4A	2.92	119.61	111.77
31	Y1	614	CLA	CMA-C3A-C4A	2.92	119.61	111.77
33	c1	516	BCR	C37-C22-C21	-2.92	118.84	122.92
31	a	410	CLA	CHD-C1D-ND	-2.91	121.78	124.45
49	R	621	XAT	C27-C28-C29	2.91	130.05	125.53
31	b1	608	CLA	CMA-C3A-C4A	2.91	119.60	111.77
31	G	612	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	S	609	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	B1	607	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	n	604	CLA	CMB-C2B-C3B	2.91	130.13	124.68
31	g1	611	CLA	CMA-C3A-C4A	2.91	119.60	111.77
47	n	601	CHL	CMA-C3A-C4A	2.91	119.60	111.77
31	y	602	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
31	g	613	CLA	C2C-C1C-NC	2.91	112.70	109.97
47	n1	606	CHL	C3C-C4C-NC	-2.91	107.31	110.57
31	N	614	CLA	C2D-C1D-ND	2.91	112.25	110.10
47	n	606	CHL	C3C-C4C-NC	-2.91	107.31	110.57
47	y1	601	CHL	C3C-C4C-NC	-2.91	107.31	110.57
31	C	513	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
31	b	615	CLA	CHD-C1D-ND	-2.91	121.78	124.45
47	g	607	CHL	C2C-C3C-C4C	2.91	108.56	106.49
31	y1	613	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	s1	617	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
31	G	613	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	S	604	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	g1	603	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	G	613	CLA	C2C-C1C-NC	2.91	112.70	109.97
35	C1	521	LMG	O8-C28-C29	2.91	121.03	111.91
31	S	605	CLA	O2A-CGA-CBA	2.91	121.03	111.91
31	s	612	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	b1	611	CLA	CHD-C1D-ND	-2.91	121.78	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	602	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	R1	612	CLA	C2D-C1D-ND	2.91	112.25	110.10
48	S	620	LUT	C31-C30-C29	-2.91	123.16	127.31
45	F	101	HEM	C3B-C2B-C1B	2.90	108.64	106.49
31	G	611	CLA	CMA-C3A-C4A	2.90	119.58	111.77
31	r1	602	CLA	CMA-C3A-C4A	2.90	119.58	111.77
31	C1	508	CLA	C1-C2-C3	-2.90	121.02	126.04
31	b1	602	CLA	C1-C2-C3	-2.90	121.02	126.04
47	n1	605	CHL	C3C-C4C-NC	-2.90	107.31	110.57
31	G1	611	CLA	C1-C2-C3	-2.90	121.02	126.04
48	g1	620	LUT	C7-C8-C9	-2.90	121.85	126.23
31	c	506	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	g1	604	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	Y1	608	CLA	CMA-C3A-C4A	2.90	119.57	111.77
48	g1	621	LUT	C35-C34-C33	-2.90	123.17	127.31
31	B	605	CLA	CHD-C1D-ND	-2.90	121.79	124.45
31	B1	612	CLA	CHD-C1D-ND	-2.90	121.79	124.45
31	c1	503	CLA	C2D-C1D-ND	2.90	112.24	110.10
49	Y1	622	XAT	C19-C9-C10	-2.90	118.86	122.92
41	D1	409	LHG	O8-C23-C24	2.90	121.00	111.91
31	S	602	CLA	CMA-C3A-C4A	2.90	119.56	111.77
49	G	622	XAT	O24-C25-C24	2.90	115.56	113.38
33	A	411	BCR	C23-C24-C25	-2.90	119.06	127.20
31	s	614	CLA	O2A-CGA-CBA	2.90	121.00	111.91
31	B1	610	CLA	C2C-C1C-NC	2.90	112.69	109.97
47	s1	601	CHL	CHD-C1D-ND	-2.90	121.79	124.45
47	R1	607	CHL	C3C-C4C-NC	-2.90	107.32	110.57
31	a	406	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
31	C1	512	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
31	a	406	CLA	CHD-C1D-ND	-2.90	121.79	124.45
31	b	614	CLA	CMB-C2B-C3B	2.90	130.09	124.68
31	B	613	CLA	C1-C2-C3	-2.90	121.04	126.04
31	B1	613	CLA	C1-C2-C3	-2.90	121.04	126.04
31	Y	604	CLA	C2C-C1C-NC	2.89	112.68	109.97
31	B	617	CLA	O2A-CGA-CBA	2.89	120.99	111.91
31	y1	614	CLA	C1-C2-C3	-2.89	121.04	126.04
31	N	604	CLA	CMB-C2B-C3B	2.89	130.09	124.68
31	g	612	CLA	C2D-C1D-ND	2.89	112.24	110.10
47	s	606	CHL	C2C-C3C-C4C	2.89	108.55	106.49
49	y	622	XAT	C40-C33-C34	-2.89	118.87	122.92
47	g1	609	CHL	CMA-C3A-C4A	2.89	119.55	111.77
50	Y1	623	NEX	C38-C25-C26	-2.89	117.41	122.26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Y1	622	XAT	O4-C5-C4	-2.89	111.21	113.38
31	c	501	CLA	C1-C2-C3	-2.89	121.04	126.04
31	Y1	612	CLA	C2D-C1D-ND	2.89	112.23	110.10
47	y1	606	CHL	C3C-C4C-NC	-2.89	107.33	110.57
31	N	611	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
47	y1	605	CHL	C4A-NA-C1A	2.89	108.00	106.71
31	R1	608	CLA	C2D-C1D-ND	2.89	112.23	110.10
31	y	602	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
31	y	613	CLA	CMA-C3A-C4A	2.89	119.53	111.77
50	g	623	NEX	C31-C30-C29	2.89	131.43	127.31
47	Y	601	CHL	C3C-C4C-NC	-2.89	107.33	110.57
33	c	517	BCR	C34-C9-C10	-2.89	118.88	122.92
31	R	603	CLA	CHD-C1D-ND	-2.89	121.80	124.45
31	S	602	CLA	CHD-C1D-ND	-2.89	121.80	124.45
31	b	607	CLA	CHD-C1D-ND	-2.89	121.80	124.45
47	G	601	CHL	C1-O2A-CGA	2.89	124.02	116.44
31	B1	604	CLA	C1-C2-C3	-2.89	121.05	126.04
32	a	408	PHO	O2D-CGD-O1D	-2.89	118.20	123.84
31	D	403	CLA	C1-C2-C3	-2.88	121.06	126.04
31	y	614	CLA	CHD-C1D-ND	-2.88	121.80	124.45
47	N1	609	CHL	C3C-C4C-NC	-2.88	107.34	110.57
31	s1	609	CLA	CHD-C1D-ND	-2.88	121.81	124.45
31	c1	510	CLA	C1-C2-C3	-2.88	121.06	126.04
31	B	615	CLA	C2C-C1C-NC	2.88	112.67	109.97
31	c	509	CLA	O2A-CGA-CBA	2.88	120.95	111.91
31	n	610	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
48	r1	620	LUT	C35-C34-C33	-2.88	123.20	127.31
31	S1	610	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	g	602	CLA	C2C-C1C-NC	2.88	112.67	109.97
47	n1	605	CHL	C2C-C3C-C4C	2.88	108.54	106.49
48	s1	621	LUT	C15-C14-C13	-2.88	123.20	127.31
31	g1	612	CLA	CHD-C1D-ND	-2.88	121.81	124.45
31	C	510	CLA	C2D-C1D-ND	2.88	112.22	110.10
31	Y	613	CLA	C2C-C1C-NC	2.88	112.67	109.97
49	r	622	XAT	C11-C10-C9	-2.88	123.20	127.31
31	a	407	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
31	c	502	CLA	CHD-C1D-ND	-2.88	121.81	124.45
47	y1	607	CHL	CHD-C1D-ND	-2.88	121.81	124.45
47	g1	607	CHL	CHD-C1D-ND	-2.88	121.81	124.45
31	B	603	CLA	CAC-C3C-C4C	2.88	128.54	124.81
49	g1	622	XAT	C26-C27-C28	-2.88	119.91	125.99
33	B	619	BCR	C27-C26-C25	-2.87	118.56	122.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	514	BCR	C33-C5-C4	2.87	119.14	113.62
31	r	604	CLA	C2D-C1D-ND	2.87	112.22	110.10
31	N1	604	CLA	C2D-C1D-ND	2.87	112.22	110.10
31	n1	614	CLA	C2D-C1D-ND	2.87	112.22	110.10
48	N	620	LUT	C22-C23-C24	-2.87	108.47	111.74
47	g1	609	CHL	C1B-CHB-C4A	-2.87	124.43	130.12
35	d1	411	LMG	O8-C28-C29	2.87	120.92	111.91
31	s	614	CLA	C1-O2A-CGA	2.87	123.98	116.44
31	B1	605	CLA	O2A-CGA-CBA	2.87	120.92	111.91
31	y1	614	CLA	CMA-C3A-C4A	2.87	119.49	111.77
33	b1	619	BCR	C1-C6-C5	-2.87	118.57	122.61
48	S1	620	LUT	C22-C23-C24	-2.87	108.47	111.74
47	S	608	CHL	C3C-C4C-NC	-2.87	107.35	110.57
31	C	505	CLA	C2C-C1C-NC	2.87	112.66	109.97
56	r1	626	ERG	C13-C17-C20	-2.87	115.72	119.43
31	y1	604	CLA	C2D-C1D-ND	2.87	112.22	110.10
47	G	608	CHL	CMA-C3A-C4A	2.87	119.49	111.77
31	s1	602	CLA	O2A-CGA-CBA	2.87	120.92	111.91
31	G1	604	CLA	C2D-C1D-ND	2.87	112.22	110.10
31	g	611	CLA	CMA-C3A-C4A	2.87	119.48	111.77
31	Y1	612	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
31	S1	611	CLA	C1-C2-C3	-2.87	121.08	126.04
47	n1	609	CHL	C1-O2A-CGA	2.87	123.97	116.44
48	g	620	LUT	C35-C15-C14	-2.87	117.60	123.47
31	C1	513	CLA	CMB-C2B-C3B	2.87	130.04	124.68
46	h1	101	RRX	C7-C6-C5	-2.87	114.52	121.46
31	R1	602	CLA	O1D-CGD-CBD	-2.87	118.62	124.48
50	N	623	NEX	C38-C25-C26	-2.87	117.46	122.26
40	C	519	DGD	O1G-C1A-C2A	2.87	120.90	111.91
31	S1	612	CLA	CHD-C1D-ND	-2.87	121.82	124.45
31	G1	602	CLA	CMA-C3A-C4A	2.87	119.48	111.77
50	R	622	NEX	O24-C25-C38	-2.87	111.62	115.06
31	C1	511	CLA	CMA-C3A-C4A	2.87	119.47	111.77
31	C	502	CLA	CMA-C3A-C4A	2.87	119.47	111.77
31	n	614	CLA	C2C-C1C-NC	2.87	112.66	109.97
31	r	602	CLA	C2D-C1D-ND	2.86	112.22	110.10
40	C1	520	DGD	O1G-C1A-C2A	2.86	120.90	111.91
31	b1	602	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
31	c	501	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
50	Y	623	NEX	C38-C25-C26	-2.86	117.46	122.26
31	G1	604	CLA	CMA-C3A-C4A	2.86	119.47	111.77
31	g1	602	CLA	CHD-C1D-ND	-2.86	121.82	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a1	410	CLA	C1-C2-C3	-2.86	121.09	126.04
31	Y	611	CLA	CHD-C1D-ND	-2.86	121.83	124.45
47	Y	606	CHL	C3C-C4C-NC	-2.86	107.36	110.57
31	g1	603	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
48	Y1	620	LUT	C38-C25-C24	-2.86	117.44	123.56
33	d	404	BCR	C37-C22-C21	-2.86	118.92	122.92
33	C1	517	BCR	C36-C18-C17	-2.86	118.92	122.92
31	r1	608	CLA	CHD-C1D-ND	-2.86	121.83	124.45
31	b1	610	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	b1	608	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
31	c	510	CLA	C2C-C1C-NC	2.86	112.65	109.97
47	n	605	CHL	C2C-C3C-C4C	2.86	108.53	106.49
48	g1	621	LUT	C18-C5-C6	-2.86	121.32	124.53
47	n1	607	CHL	C1-C2-C3	-2.86	121.10	126.04
35	D1	411	LMG	O8-C28-C29	2.86	120.87	111.91
33	B1	619	BCR	C1-C6-C5	-2.86	118.59	122.61
31	c1	511	CLA	C2D-C1D-ND	2.86	112.21	110.10
31	B	603	CLA	C1C-C2C-C3C	-2.85	103.95	106.96
48	S1	621	LUT	C22-C23-C24	-2.85	108.49	111.74
31	C1	507	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	S1	612	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	R	603	CLA	O1D-CGD-CBD	-2.85	118.64	124.48
31	B1	610	CLA	C1-C2-C3	-2.85	121.11	126.04
31	y	610	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	Y1	610	CLA	C1D-ND-C4D	-2.85	104.31	106.33
31	R	609	CLA	C2C-C1C-NC	2.85	112.64	109.97
47	n1	601	CHL	CMA-C3A-C4A	2.85	119.44	111.77
31	r	608	CLA	C1-C2-C3	-2.85	121.11	126.04
31	c	505	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
31	Y	612	CLA	C1-C2-C3	-2.85	121.11	126.04
31	B1	604	CLA	CHD-C1D-ND	-2.85	121.83	124.45
31	G1	602	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
31	D1	403	CLA	O2A-CGA-CBA	2.85	120.86	111.91
31	A	410	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
31	S	604	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
47	n	608	CHL	C3C-C4C-NC	-2.85	107.38	110.57
31	R1	603	CLA	CHD-C1D-ND	-2.85	121.84	124.45
31	S1	603	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	Y	604	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
31	R	602	CLA	CMA-C3A-C4A	2.85	119.43	111.77
31	n	614	CLA	CMA-C3A-C4A	2.85	119.42	111.77
31	s	611	CLA	C1-C2-C3	-2.85	121.12	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n1	612	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	S	614	CLA	C1-C2-C3	-2.85	121.12	126.04
31	s	617	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
31	G1	603	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
31	d	402	CLA	CHD-C1D-ND	-2.85	121.84	124.45
47	Y1	609	CHL	C2C-C3C-C4C	2.84	108.52	106.49
31	B1	612	CLA	C1D-ND-C4D	-2.84	104.31	106.33
31	b1	613	CLA	CHD-C1D-ND	-2.84	121.84	124.45
31	S1	610	CLA	C2D-C1D-ND	2.84	112.20	110.10
31	a1	405	CLA	C1-C2-C3	-2.84	121.12	126.04
41	S1	624	LHG	C5-O7-C7	-2.84	110.79	117.79
31	R	610	CLA	CMB-C2B-C3B	2.84	130.00	124.68
31	n	610	CLA	CMA-C3A-C4A	2.84	119.42	111.77
33	B1	618	BCR	C4-C5-C6	-2.84	118.60	122.73
47	s	607	CHL	C4A-NA-C1A	2.84	107.98	106.71
31	Y	611	CLA	C1-C2-C3	-2.84	121.13	126.04
47	N	606	CHL	CMA-C3A-C4A	2.84	119.41	111.77
47	R	606	CHL	CMA-C3A-C4A	2.84	119.41	111.77
31	s1	612	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
31	b1	606	CLA	CMB-C2B-C3B	2.84	129.99	124.68
31	c1	512	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
31	C	509	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
31	B1	605	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
31	s	610	CLA	C2C-C1C-NC	2.84	112.63	109.97
31	c1	501	CLA	C2D-C1D-ND	2.84	112.20	110.10
41	y	624	LHG	C6-C5-C4	-2.84	105.07	111.79
31	y	613	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
31	A	406	CLA	CMA-C3A-C4A	2.84	119.40	111.77
49	R1	621	XAT	C38-C25-C26	-2.84	117.50	122.26
41	L	101	LHG	O8-C23-C24	2.84	120.81	111.91
47	s	608	CHL	C4D-CHA-C1A	2.84	124.70	121.25
31	Y1	612	CLA	CHD-C1D-ND	-2.84	121.85	124.45
47	g	606	CHL	CMA-C3A-C4A	2.84	119.40	111.77
32	A	409	PHO	O2D-CGD-O1D	-2.84	118.29	123.84
38	J1	101	DGA	OG1-CA1-CA2	2.84	120.81	111.91
33	D	404	BCR	C38-C26-C27	2.84	119.07	113.62
50	g	623	NEX	C19-C9-C10	-2.84	118.95	122.92
31	n	602	CLA	C2D-C1D-ND	2.84	112.19	110.10
31	n	603	CLA	C2D-C1D-ND	2.84	112.19	110.10
31	b	609	CLA	CHD-C1D-ND	-2.84	121.85	124.45
31	b1	606	CLA	O2A-CGA-CBA	2.83	120.80	111.91
31	r	610	CLA	CHD-C1D-ND	-2.83	121.85	124.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B1	611	CLA	CMA-C3A-C4A	2.83	119.39	111.77
31	C1	512	CLA	CMA-C3A-C4A	2.83	119.39	111.77
31	C	512	CLA	CHD-C1D-ND	-2.83	121.85	124.45
31	b1	602	CLA	CMA-C3A-C4A	2.83	119.39	111.77
31	B	615	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
31	b	608	CLA	C1-C2-C3	-2.83	121.14	126.04
44	D1	405	PL9	C22-C23-C24	-2.83	120.84	127.66
31	a	405	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	A1	407	CLA	C2C-C1C-NC	2.83	112.62	109.97
48	Y	621	LUT	C35-C15-C14	-2.83	117.67	123.47
48	n1	621	LUT	C35-C15-C14	-2.83	117.67	123.47
31	R	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
33	c	514	BCR	C38-C26-C25	-2.83	121.35	124.53
31	A	410	CLA	C1-C2-C3	-2.83	121.15	126.04
48	y1	621	LUT	C15-C14-C13	-2.83	123.27	127.31
31	Y1	603	CLA	C2D-C1D-ND	2.83	112.19	110.10
47	r	607	CHL	CHB-C4A-NA	2.83	128.43	124.51
31	N1	612	CLA	CHD-C1D-ND	-2.83	121.85	124.45
31	b1	604	CLA	C2C-C1C-NC	2.83	112.62	109.97
33	C	514	BCR	C23-C24-C25	-2.83	119.26	127.20
47	Y	606	CHL	C2C-C3C-C4C	2.83	108.50	106.49
31	g1	614	CLA	CHD-C1D-ND	-2.83	121.86	124.45
31	s1	604	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
31	r	603	CLA	CMA-C3A-C4A	2.83	119.37	111.77
31	c	506	CLA	CMA-C3A-C4A	2.83	119.37	111.77
31	d	403	CLA	CHD-C1D-ND	-2.83	121.86	124.45
46	h1	101	RRX	C23-C22-C21	-2.83	114.60	118.94
31	r	612	CLA	CHD-C1D-ND	-2.83	121.86	124.45
47	y	606	CHL	CHD-C1D-ND	-2.83	121.86	124.45
31	y	611	CLA	C1-C2-C3	-2.83	121.16	126.04
33	C	516	BCR	C31-C1-C6	-2.83	105.72	110.30
31	S1	605	CLA	C1-O2A-CGA	2.83	123.86	116.44
31	N	611	CLA	C2D-C1D-ND	2.83	112.19	110.10
50	Y1	623	NEX	C35-C34-C33	2.83	131.34	127.31
31	C1	507	CLA	C1-O2A-CGA	2.83	123.86	116.44
50	G	623	NEX	C5-C6-C1	2.82	122.50	119.70
31	C1	511	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
47	g	607	CHL	C3C-C4C-NC	-2.82	107.40	110.57
35	c1	521	LMG	O8-C28-C29	2.82	120.77	111.91
31	Y1	602	CLA	C2C-C1C-NC	2.82	112.62	109.97
50	r	623	NEX	C38-C25-C26	-2.82	117.53	122.26
31	b	613	CLA	C2C-C1C-NC	2.82	112.62	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	606	CLA	O2A-CGA-CBA	2.82	120.76	111.91
31	c	513	CLA	O2A-CGA-CBA	2.82	120.76	111.91
31	y	603	CLA	CHD-C1D-ND	-2.82	121.86	124.45
31	y1	603	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
35	C1	523	LMG	O8-C28-C29	2.82	120.76	111.91
31	C	501	CLA	C2C-C1C-NC	2.82	112.61	109.97
31	y1	602	CLA	O2A-CGA-CBA	2.82	120.76	111.91
49	G1	622	XAT	O4-C5-C4	-2.82	111.26	113.38
31	c	512	CLA	CHD-C1D-ND	-2.82	121.86	124.45
31	C1	501	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
33	B	619	BCR	C23-C22-C21	2.82	123.27	118.94
31	b1	615	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
31	G1	604	CLA	CHD-C1D-ND	-2.82	121.86	124.45
31	B	609	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
31	y1	612	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
33	D	404	BCR	C27-C26-C25	-2.82	118.64	122.73
31	G1	613	CLA	C2D-C1D-ND	2.82	112.18	110.10
47	n	607	CHL	C4A-NA-C1A	2.82	107.97	106.71
47	N1	608	CHL	C1B-CHB-C4A	-2.82	124.54	130.12
31	a1	410	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
54	i1	101	4RF	O40-C41-C43	2.82	120.75	111.91
31	B	606	CLA	C2C-C1C-NC	2.82	112.61	109.97
31	n1	602	CLA	C2D-C1D-ND	2.82	112.18	110.10
45	f1	101	HEM	C4B-CHC-C1C	2.81	126.27	122.56
31	B	615	CLA	C1-O2A-CGA	2.81	123.83	116.44
31	b	615	CLA	CAC-C3C-C4C	2.81	128.46	124.81
31	b	613	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
41	S	624	LHG	O8-C23-C24	2.81	120.74	111.91
47	R	607	CHL	CHB-C4A-NA	2.81	128.40	124.51
47	Y	606	CHL	CHB-C4A-NA	2.81	128.40	124.51
31	c1	503	CLA	C1-C2-C3	-2.81	121.18	126.04
31	c	512	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
31	G	612	CLA	CMA-C3A-C4A	2.81	119.33	111.77
31	b1	610	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
48	n	620	LUT	C15-C14-C13	-2.81	123.30	127.31
31	G1	603	CLA	CMA-C3A-C4A	2.81	119.33	111.77
31	n1	603	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
33	b1	619	BCR	C15-C14-C13	-2.81	123.30	127.31
31	S1	605	CLA	O2A-CGA-CBA	2.81	120.73	111.91
48	y	620	LUT	C38-C25-C24	-2.81	117.54	123.56
31	a1	407	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
50	R1	622	NEX	O24-C25-C38	-2.81	111.69	115.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g1	614	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
31	r1	603	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
31	S	602	CLA	C2D-C1D-ND	2.81	112.17	110.10
31	b1	611	CLA	C1-C2-C3	-2.81	121.19	126.04
31	b	617	CLA	O2A-CGA-CBA	2.81	120.72	111.91
31	r	610	CLA	C1-C2-C3	-2.81	121.19	126.04
31	B1	609	CLA	C1-C2-C3	-2.81	121.19	126.04
40	C	520	DGD	O1G-C1A-C2A	2.81	120.72	111.91
31	c	511	CLA	C2D-C1D-ND	2.81	112.17	110.10
31	B	606	CLA	C1-C2-C3	-2.81	121.19	126.04
31	b1	609	CLA	CHA-C4D-ND	2.81	138.37	132.50
31	A1	406	CLA	O2A-CGA-CBA	2.81	120.71	111.91
47	Y	607	CHL	CHB-C4A-NA	2.80	128.39	124.51
48	S	621	LUT	C35-C15-C14	-2.80	117.73	123.47
31	c1	508	CLA	CMA-C3A-C4A	2.80	119.30	111.77
48	N1	620	LUT	C10-C11-C12	-2.80	114.47	123.22
31	s1	602	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
31	B1	609	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
31	C1	502	CLA	C1-C2-C3	-2.80	121.20	126.04
31	G	610	CLA	O1D-CGD-CBD	-2.80	118.76	124.48
31	R	610	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	S	603	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	B1	602	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	a1	405	CLA	CMC-C2C-C1C	2.80	129.30	125.04
33	c	514	BCR	C34-C9-C10	-2.80	119.00	122.92
48	r	620	LUT	C22-C23-C24	-2.80	108.56	111.74
47	Y	606	CHL	CMA-C3A-C4A	2.80	119.29	111.77
47	g	609	CHL	C3C-C4C-NC	-2.80	107.43	110.57
31	r1	612	CLA	C1-C2-C3	-2.80	121.21	126.04
31	s	605	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
31	b1	608	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	C	503	CLA	C2C-C1C-NC	2.80	112.59	109.97
31	s1	605	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
47	n1	607	CHL	C4A-NA-C1A	2.80	107.96	106.71
31	S1	602	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	b1	614	CLA	CMB-C2B-C3B	2.79	129.91	124.68
50	y	623	NEX	C16-C1-C6	-2.79	107.97	110.47
50	S1	623	NEX	C19-C9-C10	-2.79	119.01	122.92
31	B	616	CLA	CHD-C1D-ND	-2.79	121.89	124.45
50	R	622	NEX	C27-C28-C29	-2.79	121.20	125.53
31	A	405	CLA	C6-C5-C3	-2.79	106.13	113.45
31	S	603	CLA	C1-C2-C3	-2.79	121.21	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	616	CLA	C2D-C1D-ND	2.79	112.16	110.10
31	Y	603	CLA	CMA-C3A-C4A	2.79	119.28	111.77
31	S	611	CLA	CHD-C1D-ND	-2.79	121.89	124.45
47	n	607	CHL	CHB-C4A-NA	2.79	128.37	124.51
31	G1	611	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
31	n	602	CLA	CMB-C2B-C3B	2.79	129.90	124.68
31	N1	610	CLA	C2D-C1D-ND	2.79	112.16	110.10
50	r	623	NEX	C39-C29-C30	-2.79	119.01	122.92
31	b	613	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
31	y1	604	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
31	R1	610	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
31	B1	603	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
47	N	607	CHL	C1-C2-C3	-2.79	121.22	126.04
31	b	607	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
31	Y1	614	CLA	CHD-C1D-ND	-2.79	121.89	124.45
32	a1	409	PHO	O2D-CGD-O1D	-2.79	118.39	123.84
31	C1	508	CLA	C1D-ND-C4D	-2.79	104.36	106.33
47	N1	609	CHL	CHD-C1D-ND	-2.79	121.89	124.45
31	C1	505	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
49	N	622	XAT	O24-C25-C24	2.79	115.47	113.38
31	s1	609	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	n	612	CLA	C2D-C1D-ND	2.79	112.16	110.10
31	g1	612	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
31	a	410	CLA	CMB-C2B-C3B	2.79	129.89	124.68
31	s	605	CLA	CHD-C1D-ND	-2.78	121.89	124.45
31	Y	614	CLA	CMA-C3A-C4A	2.78	119.26	111.77
31	n	603	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
31	S	614	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
47	y	601	CHL	C1-O2A-CGA	2.78	123.75	116.44
31	A1	410	CLA	C1-C2-C3	-2.78	121.23	126.04
31	C1	506	CLA	CMA-C3A-C4A	2.78	119.25	111.77
31	N1	603	CLA	C2D-C1D-ND	2.78	112.16	110.10
31	b1	607	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
31	B	602	CLA	C1-C2-C3	-2.78	121.23	126.04
31	c	508	CLA	C2C-C1C-NC	2.78	112.58	109.97
31	B	602	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
31	N	614	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
31	b	616	CLA	CHD-C1D-ND	-2.78	121.90	124.45
31	G1	614	CLA	CMA-C3A-C4A	2.78	119.25	111.77
49	n	622	XAT	C19-C9-C10	-2.78	119.03	122.92
31	S	617	CLA	C2D-C1D-ND	2.78	112.15	110.10
31	S	609	CLA	C2C-C1C-NC	2.78	112.58	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	602	CLA	C1-C2-C3	-2.78	121.23	126.04
31	C1	508	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
32	A1	409	PHO	O2D-CGD-O1D	-2.78	118.40	123.84
41	S	624	LHG	C5-O7-C7	-2.78	110.94	117.79
31	A	405	CLA	C1-C2-C3	-2.78	121.23	126.04
31	s1	603	CLA	C2D-C1D-ND	2.78	112.15	110.10
31	B	613	CLA	CHD-C1D-ND	-2.78	121.90	124.45
31	c	508	CLA	CHD-C1D-ND	-2.78	121.90	124.45
47	n	609	CHL	CAA-C2A-C3A	-2.78	105.17	112.78
31	b	609	CLA	CMA-C3A-C4A	2.78	119.24	111.77
48	Y1	621	LUT	C38-C25-C24	-2.78	117.61	123.56
47	y1	607	CHL	CMA-C3A-C4A	2.78	119.24	111.77
31	Y1	613	CLA	O2A-CGA-CBA	2.78	120.63	111.91
31	r1	608	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
47	G1	606	CHL	CHB-C4A-NA	2.78	128.35	124.51
31	B	615	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
47	R1	606	CHL	CMA-C3A-C4A	2.78	119.24	111.77
47	y1	609	CHL	C1-O2A-CGA	2.78	123.73	116.44
31	g1	614	CLA	C2D-C1D-ND	2.78	112.15	110.10
50	R	622	NEX	C26-C27-C28	-2.78	120.12	125.99
31	S1	614	CLA	C1-C2-C3	-2.78	121.24	126.04
32	a	408	PHO	O1D-CGD-CBD	2.78	129.36	124.74
31	c1	504	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
33	D1	404	BCR	C38-C26-C25	-2.78	121.41	124.53
33	B	618	BCR	C36-C18-C17	-2.78	119.03	122.92
31	c1	508	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
31	s	613	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
31	S1	603	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
48	r1	620	LUT	C18-C5-C4	2.77	119.50	114.36
47	s	608	CHL	C1-O2A-CGA	2.77	123.72	116.44
31	n1	610	CLA	CMB-C2B-C3B	2.77	129.87	124.68
31	d	403	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
31	y1	608	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
31	B1	615	CLA	CMA-C3A-C4A	2.77	119.23	111.77
32	A	408	PHO	O2D-CGD-O1D	-2.77	118.42	123.84
31	C	511	CLA	O2A-CGA-CBA	2.77	120.61	111.91
31	b	605	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	S1	610	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
31	Y	603	CLA	C1-C2-C3	-2.77	121.25	126.04
33	C1	516	BCR	C23-C22-C21	2.77	123.19	118.94
47	Y	606	CHL	C1-C2-C3	-2.77	121.25	126.04
31	c1	512	CLA	CMA-C3A-C4A	2.77	119.22	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r1	621	XAT	C38-C25-C26	-2.77	117.62	122.26
31	c1	513	CLA	CBA-CAA-C2A	2.77	122.04	113.86
51	S	625	LPX	O3-P1-O4	2.77	125.93	112.24
47	G1	607	CHL	CHB-C4A-NA	2.77	128.34	124.51
47	Y1	606	CHL	C1-O2A-CGA	2.77	123.71	116.44
48	s1	620	LUT	C18-C5-C4	2.77	119.48	114.36
31	b1	603	CLA	C2D-C1D-ND	2.77	112.14	110.10
31	g1	614	CLA	CMA-C3A-C4A	2.77	119.21	111.77
31	g	602	CLA	O2A-CGA-CBA	2.77	120.59	111.91
50	s1	623	NEX	C38-C25-C26	-2.77	117.62	122.26
31	B	603	CLA	CMC-C2C-C1C	2.77	129.25	125.04
48	r	620	LUT	C15-C35-C34	-2.77	117.81	123.47
32	a1	409	PHO	C3D-CAD-CBD	-2.77	103.96	107.61
47	N1	607	CHL	C3C-C4C-NC	-2.77	107.47	110.57
47	s1	608	CHL	C1B-CHB-C4A	-2.77	124.64	130.12
49	G	622	XAT	C6-C7-C8	-2.77	120.14	125.99
33	c1	516	BCR	C34-C9-C10	-2.77	119.05	122.92
31	B1	609	CLA	CMA-C3A-C4A	2.77	119.21	111.77
47	G1	601	CHL	C4D-CHA-C1A	2.77	124.61	121.25
48	s	620	LUT	C18-C5-C4	2.77	119.48	114.36
31	N1	604	CLA	CHA-C4D-ND	2.76	138.28	132.50
31	N	613	CLA	CMA-C3A-C4A	2.76	119.20	111.77
31	C	512	CLA	C2D-C1D-ND	2.76	112.14	110.10
31	C1	502	CLA	C2D-C1D-ND	2.76	112.14	110.10
31	R1	610	CLA	CMA-C3A-C4A	2.76	119.20	111.77
45	F1	101	HEM	CMC-C2C-C3C	2.76	129.85	124.68
33	b	618	BCR	C33-C5-C4	2.76	118.92	113.62
31	c1	501	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
41	C1	525	LHG	O8-C23-C24	2.76	120.58	111.91
31	R	604	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
31	b	604	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
31	B1	606	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
31	g1	604	CLA	CMA-C3A-C4A	2.76	119.20	111.77
33	A	411	BCR	C38-C26-C25	-2.76	121.43	124.53
47	g	607	CHL	CMA-C3A-C4A	2.76	119.19	111.77
47	n	609	CHL	CHD-C4C-C3C	2.76	128.90	124.84
31	C1	507	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
31	S1	609	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
52	S1	626	3PH	O31-C31-C32	2.76	120.57	111.91
31	c	503	CLA	C2D-C1D-ND	2.76	112.14	110.10
31	B1	613	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
51	s	625	LPX	O3-P1-O4	2.76	125.88	112.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	614	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
31	S1	613	CLA	CHD-C1D-ND	-2.76	121.92	124.45
31	n	611	CLA	C3D-C2D-C1D	-2.76	102.07	105.83
31	s	611	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
31	R	613	CLA	C2D-C1D-ND	2.76	112.14	110.10
31	c1	510	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
35	w1	201	LMG	O8-C28-C29	2.76	120.56	111.91
31	Y1	608	CLA	CHA-C4D-ND	2.76	138.26	132.50
31	C1	509	CLA	C2D-C1D-ND	2.75	112.13	110.10
33	B1	619	BCR	C15-C14-C13	-2.75	123.38	127.31
31	y	603	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
45	f	101	HEM	C4D-ND-C1D	2.75	107.92	105.07
31	y	608	CLA	CMA-C3A-C4A	2.75	119.17	111.77
37	B	620	C7Z	C27-C28-C29	-2.75	122.08	126.23
31	A1	406	CLA	C1-C2-C3	-2.75	121.28	126.04
52	b1	624	3PH	O31-C31-C32	2.75	120.55	111.91
31	S1	611	CLA	CHD-C1D-ND	-2.75	121.92	124.45
31	s1	605	CLA	CHD-C1D-ND	-2.75	121.92	124.45
31	N1	612	CLA	C2D-C1D-ND	2.75	112.13	110.10
33	c	514	BCR	C36-C18-C17	-2.75	119.07	122.92
31	y	610	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
47	G	601	CHL	C1-C2-C3	-2.75	121.29	126.04
31	R	602	CLA	C2D-C1D-ND	2.75	112.13	110.10
31	s1	602	CLA	C1D-ND-C4D	-2.75	104.38	106.33
31	a	410	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
47	n1	606	CHL	CHD-C1D-ND	-2.75	121.93	124.45
31	A1	405	CLA	C2C-C1C-NC	2.75	112.55	109.97
31	C	513	CLA	O2A-CGA-CBA	2.75	120.53	111.91
31	b1	606	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	R1	603	CLA	C1-C2-C3	-2.75	121.29	126.04
31	B1	613	CLA	C2D-C1D-ND	2.75	112.13	110.10
31	S	617	CLA	CHD-C1D-ND	-2.75	121.93	124.45
50	n	623	NEX	O24-C25-C38	-2.75	111.76	115.06
31	G	612	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
41	D	409	LHG	C5-O7-C7	-2.75	111.03	117.79
33	b1	618	BCR	C38-C26-C27	2.75	118.89	113.62
52	i	101	3PH	O31-C31-C32	2.75	120.53	111.91
31	r1	610	CLA	C2C-C1C-NC	2.75	112.55	109.97
31	S1	617	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	n	604	CLA	OBD-CAD-C3D	-2.75	121.91	128.52
31	B	614	CLA	C1-C2-C3	-2.75	121.29	126.04
31	n1	613	CLA	CHD-C1D-ND	-2.75	121.93	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	611	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
33	A1	411	BCR	C23-C24-C25	-2.74	119.49	127.20
31	C	503	CLA	C1-C2-C3	-2.74	121.30	126.04
41	D	408	LHG	O8-C23-C24	2.74	120.52	111.91
31	B	611	CLA	CHD-C1D-ND	-2.74	121.93	124.45
47	n1	605	CHL	C1-O2A-CGA	2.74	123.64	116.44
31	B	611	CLA	CMA-C3A-C4A	2.74	119.15	111.77
47	N1	605	CHL	CMA-C3A-C4A	2.74	119.15	111.77
41	L1	101	LHG	O8-C23-C24	2.74	120.52	111.91
31	g	610	CLA	C2D-C1D-ND	2.74	112.12	110.10
35	A1	413	LMG	C8-O7-C10	-2.74	111.04	117.79
31	r1	604	CLA	C2D-C1D-ND	2.74	112.12	110.10
31	n1	603	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
31	b	611	CLA	C2C-C1C-NC	2.74	112.54	109.97
31	S1	605	CLA	CHD-C1D-ND	-2.74	121.94	124.45
33	C1	515	BCR	C15-C14-C13	-2.74	123.40	127.31
37	B	620	C7Z	C8-C7-C6	-2.74	119.51	127.20
47	g1	605	CHL	CHB-C4A-NA	2.74	128.30	124.51
31	R	612	CLA	C2D-C1D-ND	2.74	112.12	110.10
47	N	608	CHL	C2C-C3C-C4C	2.74	108.44	106.49
31	B	609	CLA	CHD-C1D-ND	-2.74	121.94	124.45
52	t1	101	3PH	O31-C31-C32	2.74	120.50	111.91
33	d1	404	BCR	C28-C27-C26	-2.74	109.19	114.08
31	Y1	608	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
35	c1	523	LMG	O8-C28-C29	2.74	120.49	111.91
31	g	613	CLA	CHD-C1D-ND	-2.74	121.94	124.45
47	N	606	CHL	CHB-C4A-NA	2.73	128.29	124.51
41	D1	409	LHG	C5-O7-C7	-2.73	111.06	117.79
31	g1	602	CLA	CMA-C3A-C4A	2.73	119.12	111.77
41	c	625	LHG	O8-C23-C24	2.73	120.49	111.91
31	C	501	CLA	CMA-C3A-C4A	2.73	119.12	111.77
47	n1	608	CHL	C4A-NA-C1A	2.73	107.94	106.71
31	A1	405	CLA	CMB-C2B-C3B	2.73	129.79	124.68
41	d1	410	LHG	C5-O7-C7	-2.73	111.06	117.79
31	B	606	CLA	C2D-C1D-ND	2.73	112.12	110.10
31	S	612	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	S1	605	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	y1	608	CLA	C2D-C1D-ND	2.73	112.12	110.10
31	S1	614	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
33	C	516	BCR	C23-C24-C25	-2.73	119.53	127.20
31	b	602	CLA	C2D-C1D-ND	2.73	112.12	110.10
49	R1	621	XAT	C6-C7-C8	-2.73	120.22	125.99

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	N1	601	CHL	CMA-C3A-C4A	2.73	119.11	111.77
44	d1	405	PL9	C20-C19-C21	2.73	119.86	115.27
31	C1	511	CLA	C1-C2-C3	-2.73	121.32	126.04
51	s1	625	LPX	O3-P1-O4	2.73	125.73	112.24
31	N1	613	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
31	C	505	CLA	O2A-CGA-CBA	2.73	120.47	111.91
47	G	607	CHL	C4A-NA-C1A	2.73	107.93	106.71
31	b	612	CLA	CHD-C1D-ND	-2.73	121.95	124.45
47	G	607	CHL	C1-O2A-CGA	2.73	123.59	116.44
31	Y1	613	CLA	C1-C2-C3	-2.73	121.33	126.04
31	b	604	CLA	CHD-C1D-ND	-2.72	121.95	124.45
31	b1	616	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	s1	610	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	C1	502	CLA	CHD-C1D-ND	-2.72	121.95	124.45
31	s	611	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	N	611	CLA	CHD-C1D-ND	-2.72	121.95	124.45
31	N1	602	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	n1	602	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	b	604	CLA	CMA-C3A-C4A	2.72	119.09	111.77
40	c1	518	DGD	O1G-C1A-C2A	2.72	120.45	111.91
31	c	510	CLA	CMD-C2D-C3D	-2.72	121.35	127.61
33	C	517	BCR	C15-C14-C13	-2.72	123.43	127.31
31	N	613	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	S	614	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	b1	614	CLA	C2D-C1D-ND	2.72	112.11	110.10
47	G1	601	CHL	CHB-C4A-NA	2.72	128.27	124.51
49	Y1	622	XAT	C26-C27-C28	-2.72	120.24	125.99
31	C1	506	CLA	C1-C2-C3	-2.72	121.34	126.04
31	C	504	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
31	S	610	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
31	N	604	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	B1	617	CLA	CHD-C1D-ND	-2.72	121.95	124.45
31	c1	503	CLA	CAC-C3C-C4C	2.72	128.34	124.81
50	s1	623	NEX	C5-C4-C3	2.72	114.96	111.75
47	N	609	CHL	C2C-C3C-C4C	2.72	108.43	106.49
31	b	616	CLA	C1-C2-C3	-2.72	121.34	126.04
47	g1	607	CHL	CHB-C4A-NA	2.72	128.27	124.51
47	N	605	CHL	C1-O2A-CGA	2.72	123.58	116.44
31	S	611	CLA	CMA-C3A-C4A	2.72	119.08	111.77
31	B1	617	CLA	C1-C2-C3	-2.72	121.34	126.04
31	N	612	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
31	r	603	CLA	C1C-C2C-C3C	-2.72	104.10	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	y1	622	XAT	C40-C33-C34	-2.72	119.12	122.92
31	c1	512	CLA	O2A-CGA-CBA	2.72	120.44	111.91
49	r	622	XAT	C8-C9-C10	2.72	123.11	118.94
31	g	602	CLA	C1D-ND-C4D	-2.72	104.41	106.33
31	s	603	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	s	605	CLA	C2D-C1D-ND	2.72	112.11	110.10
48	Y1	621	LUT	C15-C14-C13	-2.72	123.43	127.31
47	n1	607	CHL	CHD-C1D-ND	-2.72	121.96	124.45
47	Y1	601	CHL	C3C-C4C-NC	-2.72	107.53	110.57
47	n	601	CHL	C1-C2-C3	-2.72	121.35	126.04
31	B	608	CLA	CMA-C3A-C4A	2.72	119.07	111.77
31	s1	609	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
31	Y1	603	CLA	C1-C2-C3	-2.72	121.35	126.04
48	G	620	LUT	C31-C30-C29	-2.72	123.44	127.31
31	S	603	CLA	CHD-C1D-ND	-2.71	121.96	124.45
31	a	405	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
31	c	508	CLA	CMA-C3A-C4A	2.71	119.07	111.77
31	B1	604	CLA	CMA-C3A-C4A	2.71	119.07	111.77
50	r	623	NEX	C26-C27-C28	-2.71	120.26	125.99
47	R	606	CHL	CHB-C4A-NA	2.71	128.26	124.51
31	c1	504	CLA	CMA-C3A-C4A	2.71	119.06	111.77
33	C1	515	BCR	C1-C6-C5	-2.71	118.79	122.61
31	B	611	CLA	C2C-C1C-NC	2.71	112.51	109.97
31	b	609	CLA	CHA-C4D-ND	2.71	138.17	132.50
47	G	609	CHL	CHB-C4A-NA	2.71	128.26	124.51
31	c1	506	CLA	C1-C2-C3	-2.71	121.35	126.04
47	G	609	CHL	C3C-C4C-NC	-2.71	107.53	110.57
47	y1	607	CHL	C1-O2A-CGA	2.71	123.56	116.44
31	r	610	CLA	OBD-CAD-C3D	-2.71	122.00	128.52
33	C1	515	BCR	C23-C24-C25	-2.71	119.59	127.20
31	b1	607	CLA	C2C-C1C-NC	2.71	112.51	109.97
31	c1	512	CLA	C2D-C1D-ND	2.71	112.10	110.10
31	b1	604	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	N	603	CLA	CMA-C3A-C4A	2.71	119.06	111.77
41	L1	101	LHG	C5-O7-C7	-2.71	111.12	117.79
48	n1	620	LUT	C31-C30-C29	-2.71	123.44	127.31
44	d1	405	PL9	C22-C23-C24	-2.71	121.14	127.66
31	C	512	CLA	CMB-C2B-C3B	2.71	129.75	124.68
31	N1	611	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
47	y	601	CHL	CMA-C3A-C4A	2.71	119.05	111.77
47	y	605	CHL	C2C-C3C-C4C	2.71	108.42	106.49
49	y1	622	XAT	C19-C9-C10	-2.71	119.13	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n1	611	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
47	y1	601	CHL	CHB-C4A-NA	2.71	128.25	124.51
31	N1	612	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
47	N	605	CHL	C2C-C3C-C4C	2.71	108.42	106.49
31	G	610	CLA	C1D-ND-C4D	-2.71	104.41	106.33
49	Y	622	XAT	C7-C8-C9	-2.71	121.33	125.53
31	C	506	CLA	C1-C2-C3	-2.71	121.36	126.04
31	N	613	CLA	C2C-C1C-NC	2.70	112.51	109.97
31	b	607	CLA	CHA-C4D-ND	2.70	138.16	132.50
31	Y1	614	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	s1	605	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	s1	614	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	B	612	CLA	C1-C2-C3	-2.70	121.37	126.04
31	s	602	CLA	CHD-C1D-ND	-2.70	121.97	124.45
41	c1	525	LHG	O8-C23-C24	2.70	120.39	111.91
31	R	612	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	s	611	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	b1	613	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	b1	614	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	a1	405	CLA	CAC-C3C-C4C	2.70	128.32	124.81
31	G1	610	CLA	C2C-C1C-NC	2.70	112.50	109.97
31	G	604	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
47	g	609	CHL	CHB-C4A-NA	2.70	128.25	124.51
31	B	610	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
31	b1	613	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
31	C	505	CLA	C1-O2A-CGA	2.70	123.53	116.44
31	c1	509	CLA	C2D-C1D-ND	2.70	112.09	110.10
31	r	608	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
41	d1	408	LHG	O8-C23-C24	2.70	120.39	111.91
31	A	410	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
57	y1	626	PTY	O4-C30-C31	2.70	120.38	111.91
31	C1	503	CLA	CHA-C4D-ND	2.70	138.15	132.50
47	R1	607	CHL	C1-O2A-CGA	2.70	123.53	116.44
31	Y	602	CLA	C2D-C1D-ND	2.70	112.09	110.10
31	g1	610	CLA	C2D-C1D-ND	2.70	112.09	110.10
31	B	609	CLA	CHA-C4D-ND	2.70	138.15	132.50
31	d1	403	CLA	CMA-C3A-C4A	2.70	119.03	111.77
47	G1	607	CHL	C1-O2A-CGA	2.70	123.53	116.44
47	G1	608	CHL	C4D-CHA-C1A	2.70	124.53	121.25
31	a	410	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	A1	410	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
33	C	516	BCR	C37-C22-C23	2.70	122.33	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	F	101	HEM	C4C-CHD-C1D	2.70	126.12	122.56
31	B	612	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
33	C1	514	BCR	C33-C5-C4	2.70	118.80	113.62
33	c1	514	BCR	C33-C5-C4	2.70	118.80	113.62
31	c	502	CLA	C2C-C1C-NC	2.70	112.50	109.97
31	n	602	CLA	C2C-C1C-NC	2.70	112.50	109.97
31	c	513	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
31	s1	609	CLA	C2D-C1D-ND	2.70	112.09	110.10
33	C	515	BCR	C23-C24-C25	-2.70	119.63	127.20
31	Y	614	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	D1	403	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
47	N1	601	CHL	C1B-CHB-C4A	-2.70	124.78	130.12
31	Y	604	CLA	C2D-C1D-ND	2.69	112.09	110.10
44	d1	405	PL9	C40-C39-C41	2.69	119.80	115.27
35	B1	622	LMG	O8-C28-C29	2.69	120.36	111.91
41	d1	410	LHG	O8-C23-C24	2.69	120.36	111.91
31	g	614	CLA	C2D-C1D-ND	2.69	112.09	110.10
31	c1	506	CLA	CMA-C3A-C4A	2.69	119.01	111.77
48	N1	620	LUT	C7-C8-C9	-2.69	122.17	126.23
47	s	608	CHL	C3C-C4C-NC	-2.69	107.55	110.57
31	B1	611	CLA	O2A-CGA-CBA	2.69	120.36	111.91
31	s	612	CLA	CMA-C3A-C4A	2.69	119.01	111.77
44	D1	405	PL9	C20-C19-C21	2.69	119.80	115.27
31	b1	602	CLA	C2D-C1D-ND	2.69	112.09	110.10
47	s	608	CHL	C1B-CHB-C4A	-2.69	124.78	130.12
50	R	622	NEX	C40-C33-C34	-2.69	119.15	122.92
50	y1	623	NEX	C38-C25-C26	-2.69	117.75	122.26
31	n	611	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
31	n	610	CLA	C1D-ND-C4D	-2.69	104.42	106.33
35	A	413	LMG	O8-C28-C29	2.69	120.35	111.91
31	b1	609	CLA	CHD-C1D-ND	-2.69	121.98	124.45
31	a1	407	CLA	O1D-CGD-CBD	-2.69	118.98	124.48
31	y1	613	CLA	C2D-C1D-ND	2.69	112.09	110.10
31	c1	507	CLA	O2A-CGA-CBA	2.69	120.35	111.91
50	g1	623	NEX	C4-C3-C2	2.69	115.97	110.77
31	b	608	CLA	CMA-C3A-C4A	2.69	119.00	111.77
31	b1	605	CLA	CMA-C3A-C4A	2.69	119.00	111.77
41	n1	624	LHG	O8-C23-C24	2.69	120.35	111.91
31	S	610	CLA	C1-C2-C3	-2.69	121.39	126.04
31	n	602	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
31	Y	612	CLA	CHD-C1D-ND	-2.69	121.98	124.45
48	N1	620	LUT	C18-C5-C6	-2.69	121.51	124.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	617	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
37	b1	620	C7Z	C28-C27-C26	-2.69	119.65	127.20
47	S1	601	CHL	CHB-C4A-NA	2.69	128.23	124.51
31	y	610	CLA	C2D-C1D-ND	2.69	112.08	110.10
31	B1	602	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	d	403	CLA	O2A-CGA-CBA	2.69	120.34	111.91
48	Y	620	LUT	C10-C11-C12	-2.69	114.84	123.22
31	b1	608	CLA	CMB-C2B-C1B	-2.69	124.34	128.46
31	S1	611	CLA	CMA-C3A-C4A	2.68	118.99	111.77
31	b	615	CLA	CHA-C4D-ND	2.68	138.12	132.50
50	Y	623	NEX	C4-C3-C2	2.68	115.96	110.77
31	c1	511	CLA	C2C-C1C-NC	2.68	112.49	109.97
31	n1	604	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
52	B1	624	3PH	O31-C31-C32	2.68	120.33	111.91
31	B	616	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
31	B	609	CLA	CMB-C2B-C3B	2.68	129.70	124.68
31	y	602	CLA	CMA-C3A-C4A	2.68	118.98	111.77
41	d	408	LHG	O8-C23-C24	2.68	120.33	111.91
47	R	607	CHL	CMA-C3A-C4A	2.68	118.98	111.77
31	g1	602	CLA	C1-C2-C3	-2.68	121.40	126.04
54	k1	101	4RF	O18-C16-C15	2.68	120.33	111.91
31	S1	604	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
31	r	602	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
48	S1	621	LUT	C38-C25-C24	-2.68	117.82	123.56
46	h	101	RRX	C8-C7-C6	-2.68	119.67	127.20
31	Y	611	CLA	C2D-C1D-ND	2.68	112.08	110.10
31	n1	603	CLA	C2D-C1D-ND	2.68	112.08	110.10
31	N	604	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
31	G1	614	CLA	CHD-C1D-ND	-2.68	121.99	124.45
47	g1	608	CHL	C2C-C3C-C4C	2.68	108.40	106.49
31	r	610	CLA	C2C-C1C-NC	2.68	112.48	109.97
31	c	505	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
33	a1	411	BCR	C33-C5-C4	2.68	118.76	113.62
48	Y	620	LUT	C38-C25-C24	-2.68	117.83	123.56
31	Y1	603	CLA	CHD-C1D-ND	-2.68	121.99	124.45
32	A1	409	PHO	O1D-CGD-CBD	2.68	129.20	124.74
48	G	621	LUT	C22-C23-C24	-2.68	108.69	111.74
47	y	601	CHL	CHB-C4A-NA	2.68	128.21	124.51
47	G	606	CHL	CHB-C4A-NA	2.67	128.21	124.51
31	S	605	CLA	C2D-C1D-ND	2.67	112.08	110.10
47	g	609	CHL	C1-O2A-CGA	2.67	123.46	116.44
48	N1	621	LUT	C38-C25-C24	-2.67	117.84	123.56

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A1	406	CLA	C2C-C1C-NC	2.67	112.48	109.97
31	c1	506	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	y1	614	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
51	S1	625	LPX	O3-P1-O4	2.67	125.45	112.24
31	B1	615	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
48	n1	621	LUT	C31-C30-C29	-2.67	123.50	127.31
31	s	613	CLA	CHA-C4D-ND	2.67	138.09	132.50
47	N1	609	CHL	C4A-NA-C1A	2.67	107.91	106.71
31	B1	614	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	B1	616	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	b1	603	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	B	609	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
31	C	501	CLA	CHA-C4D-ND	2.67	138.09	132.50
31	B1	609	CLA	CMB-C2B-C3B	2.67	129.67	124.68
31	s	605	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
40	C	518	DGD	O1G-C1A-C2A	2.67	120.29	111.91
31	n	613	CLA	C2C-C1C-NC	2.67	112.47	109.97
31	r1	602	CLA	C2C-C1C-NC	2.67	112.47	109.97
31	B1	606	CLA	CHA-C4D-ND	2.67	138.08	132.50
47	Y	601	CHL	CHB-C4A-NA	2.67	128.20	124.51
47	n1	607	CHL	C1-O2A-CGA	2.67	123.45	116.44
31	C	511	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	g1	612	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	C	504	CLA	C1D-ND-C4D	-2.67	104.44	106.33
47	g	607	CHL	CHB-C4A-NA	2.67	128.20	124.51
49	r	622	XAT	C18-C5-C6	-2.67	117.79	122.26
41	n1	624	LHG	C5-O7-C7	-2.67	111.22	117.79
31	D1	402	CLA	C1D-ND-C4D	-2.67	104.44	106.33
47	G1	609	CHL	C1B-CHB-C4A	-2.67	124.83	130.12
31	y	608	CLA	CMD-C2D-C3D	-2.67	121.48	127.61
31	y	611	CLA	CMA-C3A-C4A	2.67	118.94	111.77
33	c	514	BCR	C40-C30-C25	-2.67	105.97	110.30
47	N	609	CHL	C1-O2A-CGA	2.67	123.44	116.44
31	b	610	CLA	C1-C2-C3	-2.67	121.43	126.04
31	C1	503	CLA	C1-C2-C3	-2.67	121.43	126.04
47	S1	608	CHL	C1-C2-C3	-2.67	121.43	126.04
31	c1	513	CLA	C2C-C1C-NC	2.67	112.47	109.97
31	y1	602	CLA	CMA-C3A-C4A	2.67	118.94	111.77
31	b	612	CLA	C1-C2-C3	-2.67	121.43	126.04
31	C	501	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
40	c	519	DGD	O1G-C1A-C2A	2.67	120.27	111.91
33	a	411	BCR	C36-C18-C17	-2.66	119.19	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B1	623	DGD	O1G-C1A-C2A	2.66	120.27	111.91
41	s1	624	LHG	O8-C23-C24	2.66	120.27	111.91
31	R1	602	CLA	C1-C2-C3	-2.66	121.44	126.04
31	r	609	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
33	C	516	BCR	C36-C18-C17	-2.66	119.19	122.92
31	b	610	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
31	c	504	CLA	C1-O2A-CGA	2.66	123.43	116.44
31	Y	613	CLA	CHD-C1D-ND	-2.66	122.01	124.45
47	R1	606	CHL	CHB-C4A-NA	2.66	128.19	124.51
31	B1	609	CLA	C2D-C1D-ND	2.66	112.07	110.10
49	g	622	XAT	C26-C27-C28	-2.66	120.36	125.99
48	s	621	LUT	C35-C34-C33	-2.66	123.51	127.31
49	n1	622	XAT	C7-C8-C9	-2.66	121.40	125.53
31	S	603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	G	602	CLA	C2C-C1C-NC	2.66	112.47	109.97
31	b1	617	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	g1	610	CLA	CMA-C3A-C4A	2.66	118.92	111.77
48	Y	621	LUT	C18-C5-C6	-2.66	121.54	124.53
35	D	411	LMG	O8-C28-C29	2.66	120.26	111.91
31	B	615	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	Y1	602	CLA	O2A-CGA-CBA	2.66	120.26	111.91
31	g1	614	CLA	O2A-CGA-CBA	2.66	120.26	111.91
50	G1	623	NEX	C38-C25-C26	-2.66	117.80	122.26
47	n1	607	CHL	C3C-C4C-NC	-2.66	107.59	110.57
31	G	614	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	r1	603	CLA	C1-C2-C3	-2.66	121.44	126.04
31	G	612	CLA	C2D-C1D-ND	2.66	112.06	110.10
31	b	608	CLA	C2D-C1D-ND	2.66	112.06	110.10
56	R1	626	ERG	C2-C3-C4	2.66	113.95	110.31
31	g	612	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
31	g1	613	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
47	G1	606	CHL	CMA-C3A-C4A	2.66	118.92	111.77
31	c	505	CLA	CHA-C4D-ND	2.66	138.06	132.50
31	B	605	CLA	C2D-C1D-ND	2.66	112.06	110.10
47	y	607	CHL	C1-O2A-CGA	2.66	123.42	116.44
31	y	603	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	y1	611	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	G	614	CLA	C2D-C1D-ND	2.66	112.06	110.10
31	B1	612	CLA	CMA-C3A-C4A	2.66	118.91	111.77
31	b1	610	CLA	CHA-C4D-ND	2.66	138.06	132.50
31	a1	410	CLA	O2A-CGA-CBA	2.66	120.24	111.91
31	S	602	CLA	C2C-C1C-NC	2.66	112.46	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	y	623	NEX	C28-C29-C30	2.66	123.02	118.94
38	b	623	DGA	OG1-CA1-CA2	2.66	120.24	111.91
31	r1	603	CLA	CHD-C1D-ND	-2.66	122.01	124.45
31	y	604	CLA	C1-C2-C3	-2.66	121.45	126.04
31	g	614	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	B	604	CLA	CHA-C4D-ND	2.65	138.05	132.50
31	G	602	CLA	CMA-C3A-C4A	2.65	118.91	111.77
33	b	619	BCR	C30-C25-C26	-2.65	118.88	122.61
38	C	524	DGA	OG1-CA1-CA2	2.65	120.24	111.91
31	S1	613	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
48	S1	620	LUT	C31-C30-C29	-2.65	123.52	127.31
31	B	612	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
47	S1	608	CHL	CHB-C4A-NA	2.65	128.18	124.51
31	y	604	CLA	CHD-C1D-ND	-2.65	122.02	124.45
31	B	608	CLA	C2D-C1D-ND	2.65	112.06	110.10
47	n	605	CHL	CMA-C3A-C4A	2.65	118.90	111.77
49	G1	622	XAT	O24-C25-C24	2.65	115.37	113.38
31	S1	614	CLA	CMD-C2D-C3D	-2.65	121.51	127.61
47	n1	609	CHL	C1B-CHB-C4A	-2.65	124.87	130.12
31	B1	609	CLA	CHA-C4D-ND	2.65	138.04	132.50
31	B1	610	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
31	s1	613	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	B	617	CLA	C2D-C1D-ND	2.65	112.06	110.10
31	C	506	CLA	C2D-C1D-ND	2.65	112.06	110.10
31	b1	612	CLA	CAC-C3C-C4C	2.65	128.25	124.81
31	C	509	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
31	Y1	602	CLA	C2D-C1D-ND	2.65	112.06	110.10
31	b	614	CLA	C1-C2-C3	-2.65	121.46	126.04
31	y	604	CLA	CMA-C3A-C4A	2.65	118.89	111.77
31	C1	505	CLA	CHA-C4D-ND	2.65	138.04	132.50
35	C	521	LMG	C8-O7-C10	-2.65	111.27	117.79
31	r	613	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
33	B	618	BCR	C34-C9-C10	-2.65	119.21	122.92
41	d	410	LHG	O8-C23-C24	2.65	120.22	111.91
31	c1	501	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	b1	611	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
31	B	607	CLA	CMB-C2B-C3B	2.65	129.63	124.68
31	s1	604	CLA	O2A-CGA-CBA	2.65	120.22	111.91
47	n1	606	CHL	CMA-C3A-C4A	2.65	118.89	111.77
31	Y	612	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
48	s	621	LUT	C15-C35-C34	-2.65	118.05	123.47
50	n	623	NEX	C40-C33-C34	-2.65	119.22	122.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	604	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	S	605	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
48	y	621	LUT	C31-C30-C29	-2.65	123.53	127.31
31	d1	403	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
49	N1	622	XAT	O4-C5-C4	-2.64	111.40	113.38
35	W1	201	LMG	O8-C28-C29	2.64	120.20	111.91
31	y	608	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	R1	608	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	B1	607	CLA	O2A-CGA-CBA	2.64	120.20	111.91
31	g	604	CLA	C2D-C1D-ND	2.64	112.05	110.10
54	K1	101	4RF	O18-C16-C15	2.64	120.19	111.91
31	b	603	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
32	A	409	PHO	O1D-CGD-CBD	2.64	129.14	124.74
31	c	512	CLA	CMB-C2B-C3B	2.64	129.62	124.68
31	Y1	604	CLA	CMA-C3A-C4A	2.64	118.87	111.77
47	Y1	607	CHL	CMA-C3A-C4A	2.64	118.87	111.77
31	Y	612	CLA	O2A-CGA-CBA	2.64	120.19	111.91
31	C	513	CLA	CMA-C3A-C4A	2.64	118.87	111.77
31	c	504	CLA	C1D-ND-C4D	-2.64	104.46	106.33
31	g1	612	CLA	CMA-C3A-C4A	2.64	118.86	111.77
47	G	601	CHL	CHB-C4A-NA	2.64	128.16	124.51
31	s1	603	CLA	CHD-C1D-ND	-2.64	122.03	124.45
31	a1	410	CLA	CMA-C3A-C4A	2.64	118.86	111.77
31	b	613	CLA	CHA-C4D-ND	2.64	138.02	132.50
33	C	517	BCR	C28-C27-C26	-2.64	109.37	114.08
31	C1	509	CLA	CMA-C3A-C4A	2.64	118.86	111.77
54	k1	101	4RF	O40-C41-C43	2.64	120.18	111.91
31	Y	610	CLA	O2A-CGA-CBA	2.64	120.18	111.91
33	c1	515	BCR	C33-C5-C4	2.64	118.68	113.62
31	n	604	CLA	C2C-C1C-NC	2.64	112.44	109.97
31	B	603	CLA	C2D-C1D-ND	2.64	112.05	110.10
31	b	612	CLA	C1D-ND-C4D	-2.64	104.46	106.33
31	G	613	CLA	CMC-C2C-C1C	2.64	129.05	125.04
48	N	621	LUT	C38-C25-C24	-2.64	117.92	123.56
33	d1	404	BCR	C36-C18-C17	-2.64	119.23	122.92
45	F	101	HEM	C4D-ND-C1D	2.64	107.80	105.07
31	b	602	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
31	s1	603	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
31	b	607	CLA	O1D-CGD-CBD	-2.64	119.09	124.48
35	C	521	LMG	O8-C28-C29	2.64	120.18	111.91
31	n	603	CLA	CMA-C3A-C4A	2.64	118.86	111.77
31	Y1	604	CLA	C1C-C2C-C3C	-2.64	104.19	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B1	607	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
47	n	605	CHL	C1-O2A-CGA	2.63	123.36	116.44
31	y1	613	CLA	C1-C2-C3	-2.63	121.49	126.04
31	b1	617	CLA	CHD-C1D-ND	-2.63	122.03	124.45
47	N1	601	CHL	C4D-CHA-C1A	2.63	124.45	121.25
31	b1	605	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
47	N1	609	CHL	C1-O2A-CGA	2.63	123.36	116.44
31	S	605	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	B	602	CLA	C2D-C1D-ND	2.63	112.05	110.10
31	B1	616	CLA	C2D-C1D-ND	2.63	112.05	110.10
31	G1	612	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
33	c1	515	BCR	C23-C24-C25	-2.63	119.81	127.20
47	n1	608	CHL	CHB-C4A-NA	2.63	128.15	124.51
31	b	615	CLA	CMA-C3A-C4A	2.63	118.85	111.77
31	b	617	CLA	CMA-C3A-C4A	2.63	118.85	111.77
31	r	613	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	c1	506	CLA	C2D-C1D-ND	2.63	112.04	110.10
31	g	613	CLA	C1D-ND-C4D	-2.63	104.47	106.33
42	C1	527	LMK	O3-C4-C3	-2.63	113.95	122.98
50	S	622	NEX	C38-C25-C26	-2.63	117.85	122.26
31	c	513	CLA	C2C-C1C-NC	2.63	112.44	109.97
31	r	609	CLA	C2D-C1D-ND	2.63	112.04	110.10
35	h	102	LMG	O8-C28-C29	2.63	120.16	111.91
31	C	501	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
31	b1	608	CLA	CHA-C4D-ND	2.63	138.00	132.50
31	c1	505	CLA	CHA-C4D-ND	2.63	138.00	132.50
31	D1	403	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
31	y	612	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
40	c	518	DGD	O1G-C1A-C2A	2.63	120.16	111.91
47	n1	601	CHL	CHB-C4A-NA	2.63	128.15	124.51
47	Y	607	CHL	CMA-C3A-C4A	2.63	118.84	111.77
31	r	612	CLA	C2D-C1D-ND	2.63	112.04	110.10
47	s	608	CHL	C4A-NA-C1A	2.63	107.89	106.71
31	r	608	CLA	CHA-C4D-ND	2.63	137.99	132.50
31	C1	512	CLA	O2A-CGA-CBA	2.63	120.15	111.91
48	s1	621	LUT	C18-C5-C4	2.63	119.22	114.36
32	a1	409	PHO	O1D-CGD-CBD	2.63	129.11	124.74
48	s1	621	LUT	C35-C15-C14	-2.63	118.09	123.47
31	A	410	CLA	C2D-C1D-ND	2.63	112.04	110.10
31	c	510	CLA	C2D-C1D-ND	2.63	112.04	110.10
31	s1	604	CLA	C2D-C1D-ND	2.63	112.04	110.10
31	G1	610	CLA	CMA-C3A-C4A	2.63	118.83	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	J	101	LMG	O8-C28-C29	2.63	120.15	111.91
31	B1	608	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
31	S1	604	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
48	N1	621	LUT	C18-C5-C6	-2.63	121.58	124.53
47	s1	601	CHL	C3C-C4C-NC	-2.63	107.63	110.57
31	C	511	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	y1	608	CLA	CMA-C3A-C4A	2.62	118.83	111.77
31	B	607	CLA	CHA-C4D-ND	2.62	137.99	132.50
31	b	615	CLA	CMB-C2B-C3B	2.62	129.59	124.68
31	R	613	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
48	r1	620	LUT	C15-C35-C34	-2.62	118.10	123.47
47	S	608	CHL	C2C-C3C-C4C	2.62	108.36	106.49
31	S	613	CLA	C1-C2-C3	-2.62	121.51	126.04
31	s1	613	CLA	C2D-C1D-ND	2.62	112.04	110.10
31	y1	610	CLA	C2D-C1D-ND	2.62	112.04	110.10
31	S1	602	CLA	C2C-C1C-NC	2.62	112.43	109.97
31	g1	613	CLA	C1-C2-C3	-2.62	121.51	126.04
31	R	602	CLA	CMB-C2B-C3B	2.62	129.59	124.68
31	s1	610	CLA	CMA-C3A-C4A	2.62	118.82	111.77
35	A	413	LMG	C8-O7-C10	-2.62	111.33	117.79
31	b	614	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
31	a	406	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	g1	614	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	C	509	CLA	C2D-C1D-ND	2.62	112.04	110.10
31	N	613	CLA	C1-C2-C3	-2.62	121.51	126.04
47	n	605	CHL	C1B-CHB-C4A	-2.62	124.92	130.12
31	b1	604	CLA	CMC-C2C-C1C	2.62	129.03	125.04
31	C	504	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
31	N	610	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
31	g1	611	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
41	s	624	LHG	O8-C23-C24	2.62	120.13	111.91
31	s1	617	CLA	O2A-CGA-CBA	2.62	120.13	111.91
52	T1	101	3PH	O31-C31-C32	2.62	120.13	111.91
50	S1	623	NEX	C1-C2-C3	2.62	119.56	113.64
31	c	508	CLA	C2D-C1D-ND	2.62	112.03	110.10
47	N1	601	CHL	C1-C2-C3	-2.62	121.51	126.04
31	B1	610	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	R1	603	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	g	611	CLA	CHD-C1D-ND	-2.62	122.05	124.45
31	Y	604	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	n	603	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
48	y1	620	LUT	C38-C25-C24	-2.62	117.96	123.56

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G1	602	CLA	C2C-C1C-NC	2.62	112.42	109.97
40	c	523	DGD	O1G-C1A-C2A	2.62	120.12	111.91
31	r1	609	CLA	CHD-C1D-ND	-2.62	122.05	124.45
31	A1	405	CLA	C2D-C1D-ND	2.62	112.03	110.10
31	n	613	CLA	CMC-C2C-C1C	2.62	129.03	125.04
46	h	101	RRX	C21-C20-C19	-2.62	115.05	123.22
31	S	610	CLA	CHA-C4D-ND	2.62	137.97	132.50
31	C	513	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
31	S1	602	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
50	N	623	NEX	C4-C3-C2	2.62	115.83	110.77
49	N1	622	XAT	C18-C5-C6	-2.62	117.88	122.26
31	s	609	CLA	C2D-C1D-ND	2.62	112.03	110.10
31	B1	617	CLA	C2D-C1D-ND	2.62	112.03	110.10
56	r1	626	ERG	C6-C7-C8	-2.62	116.92	122.07
31	G	604	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
31	S	613	CLA	CHA-C4D-ND	2.62	137.97	132.50
31	C1	501	CLA	C1-C2-C3	-2.62	121.52	126.04
31	y	603	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
31	R	611	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
50	S	622	NEX	C19-C9-C10	-2.61	119.26	122.92
31	R1	602	CLA	CMA-C3A-C4A	2.61	118.80	111.77
31	B	605	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	g	611	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	G	610	CLA	O2A-CGA-CBA	2.61	120.11	111.91
33	B1	618	BCR	C36-C18-C17	-2.61	119.26	122.92
35	j	101	LMG	O8-C28-C29	2.61	120.11	111.91
31	S	610	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
31	c	503	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	Y1	608	CLA	CMD-C2D-C3D	-2.61	121.60	127.61
31	B	615	CLA	CHA-C4D-ND	2.61	137.96	132.50
31	c1	505	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	N1	614	CLA	C1D-ND-C4D	-2.61	104.48	106.33
47	y	606	CHL	C1-O2A-CGA	2.61	123.30	116.44
31	B	610	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	c	501	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	R1	609	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	S	612	CLA	CMA-C3A-C4A	2.61	118.79	111.77
31	d1	403	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
31	G1	610	CLA	O2A-CGA-CBA	2.61	120.10	111.91
31	G1	614	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
31	B	605	CLA	CHA-C4D-ND	2.61	137.96	132.50
31	B1	608	CLA	CMD-C2D-C3D	-2.61	121.61	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R1	612	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	C1	501	CLA	CMD-C2D-C3D	-2.61	121.61	127.61
54	i1	101	4RF	O18-C16-C15	2.61	120.10	111.91
31	Y	603	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
31	b	606	CLA	C1-C2-C3	-2.61	121.53	126.04
31	b	608	CLA	O2A-CGA-CBA	2.61	120.10	111.91
50	r1	622	NEX	C16-C1-C6	-2.61	108.14	110.47
50	n1	623	NEX	C38-C25-C26	-2.61	117.89	122.26
31	c1	513	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
33	b	618	BCR	C23-C24-C25	-2.61	119.88	127.20
31	N1	614	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	d	402	CLA	CMC-C2C-C1C	2.61	129.01	125.04
31	N	612	CLA	C2D-C1D-ND	2.61	112.03	110.10
31	a	406	CLA	C2D-C1D-ND	2.61	112.03	110.10
31	d1	403	CLA	O2A-CGA-CBA	2.61	120.09	111.91
48	g	620	LUT	C38-C25-C24	-2.61	117.98	123.56
47	n1	601	CHL	C1-O2A-CGA	2.61	123.29	116.44
31	c	510	CLA	CHA-C4D-ND	2.61	137.95	132.50
31	n	604	CLA	CHD-C1D-ND	-2.61	122.06	124.45
31	R1	602	CLA	CHD-C1D-ND	-2.61	122.06	124.45
31	b1	616	CLA	C2D-C1D-ND	2.61	112.03	110.10
47	G	601	CHL	C2C-C3C-C4C	2.61	108.35	106.49
31	G	611	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
31	c1	510	CLA	O2A-CGA-CBA	2.61	120.08	111.91
31	s	611	CLA	CMA-C3A-C4A	2.61	118.78	111.77
31	n1	603	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
31	b	616	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
31	y1	611	CLA	CHA-C4D-ND	2.61	137.95	132.50
33	c1	514	BCR	C36-C18-C17	-2.60	119.27	122.92
31	a1	410	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	C1	513	CLA	CMA-C3A-C4A	2.60	118.77	111.77
31	r1	604	CLA	CMA-C3A-C4A	2.60	118.77	111.77
31	s1	603	CLA	CHA-C4D-ND	2.60	137.95	132.50
31	b	614	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	B	613	CLA	CHA-C4D-ND	2.60	137.95	132.50
31	N1	603	CLA	CHA-C4D-ND	2.60	137.95	132.50
31	d	402	CLA	C1D-ND-C4D	-2.60	104.48	106.33
31	S	613	CLA	CHD-C1D-ND	-2.60	122.06	124.45
31	C1	513	CLA	C1D-ND-C4D	-2.60	104.49	106.33
31	n	611	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	y	604	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	r1	604	CLA	C1C-C2C-C3C	-2.60	104.22	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	503	CLA	CMD-C2D-C3D	-2.60	121.63	127.61
47	g1	607	CHL	C1-O2A-CGA	2.60	123.27	116.44
50	N	623	NEX	C17-C1-C6	-2.60	108.14	110.47
47	S	608	CHL	C4D-CHA-C1A	2.60	124.42	121.25
31	g1	611	CLA	C1-C2-C3	-2.60	121.54	126.04
31	Y	602	CLA	O2A-CGA-CBA	2.60	120.07	111.91
31	N	611	CLA	CHA-C4D-ND	2.60	137.94	132.50
48	Y	621	LUT	C38-C25-C24	-2.60	117.99	123.56
31	A1	405	CLA	CHA-C4D-ND	2.60	137.94	132.50
31	c1	507	CLA	CMA-C3A-C4A	2.60	118.76	111.77
35	H1	102	LMG	O8-C28-C29	2.60	120.07	111.91
31	Y	608	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	Y	602	CLA	CMB-C2B-C3B	2.60	129.54	124.68
41	y1	624	LHG	O8-C23-C24	2.60	120.07	111.91
32	A1	408	PHO	O2D-CGD-O1D	-2.60	118.76	123.84
31	G1	604	CLA	CMB-C2B-C3B	2.60	129.54	124.68
31	s	603	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	r	602	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
31	c1	511	CLA	CBA-CAA-C2A	2.60	121.53	113.86
45	F	101	HEM	CHC-C4B-C3B	2.60	128.55	124.57
33	c1	515	BCR	C8-C9-C10	2.60	122.93	118.94
47	N1	605	CHL	C1B-CHB-C4A	-2.60	124.97	130.12
31	n	612	CLA	C2C-C1C-NC	2.60	112.41	109.97
31	C	512	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
47	R	606	CHL	C3C-C4C-NC	-2.60	107.66	110.57
33	b1	618	BCR	C31-C1-C6	-2.60	106.09	110.30
31	G1	610	CLA	C1D-ND-C4D	-2.60	104.49	106.33
49	y	622	XAT	C18-C5-C6	-2.60	117.91	122.26
31	s1	609	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
47	n	601	CHL	CHB-C4A-NA	2.60	128.10	124.51
31	n	613	CLA	C1-O2A-CGA	2.60	123.25	116.44
31	R	609	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	c1	507	CLA	CHA-C4D-ND	2.60	137.93	132.50
31	R1	609	CLA	O2A-CGA-CBA	2.59	120.05	111.91
40	c1	520	DGD	O1G-C1A-C2A	2.59	120.05	111.91
47	n	606	CHL	C1-C2-C3	-2.59	121.56	126.04
31	r	610	CLA	CAA-C2A-C3A	-2.59	105.67	112.78
31	s1	602	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
47	n1	606	CHL	CHB-C4A-NA	2.59	128.10	124.51
31	c1	507	CLA	C2C-C1C-NC	2.59	112.40	109.97
50	s1	623	NEX	C31-C32-C33	2.59	133.70	126.42
31	r	611	CLA	C1C-C2C-C3C	-2.59	104.23	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g1	621	LUT	C15-C35-C34	-2.59	118.16	123.47
31	n	610	CLA	C1-C2-C3	-2.59	121.56	126.04
31	B1	602	CLA	CHA-C4D-ND	2.59	137.92	132.50
50	s1	623	NEX	C2-C1-C6	2.59	111.73	109.21
31	Y	612	CLA	CMA-C3A-C4A	2.59	118.74	111.77
31	s1	605	CLA	CHA-C4D-ND	2.59	137.92	132.50
31	c	509	CLA	CHA-C4D-ND	2.59	137.92	132.50
31	c	512	CLA	CHA-C4D-ND	2.59	137.92	132.50
47	y1	601	CHL	C1-C2-C3	-2.59	121.56	126.04
31	c1	512	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
33	C1	517	BCR	C38-C26-C25	-2.59	121.62	124.53
31	r	612	CLA	O2A-CGA-CBA	2.59	120.04	111.91
31	g	612	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
47	g	609	CHL	C1B-CHB-C4A	-2.59	124.99	130.12
35	h1	102	LMG	O8-C28-C29	2.59	120.04	111.91
31	s1	612	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
31	B1	607	CLA	CHA-C4D-ND	2.59	137.92	132.50
31	S1	610	CLA	CHD-C1D-ND	-2.59	122.07	124.45
31	c	501	CLA	O2A-CGA-CBA	2.59	120.03	111.91
41	d	409	LHG	O8-C23-C24	2.59	120.03	111.91
33	c1	516	BCR	C33-C5-C4	2.59	118.59	113.62
31	b1	613	CLA	CMD-C2D-C3D	-2.59	121.66	127.61
31	b	608	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	s1	602	CLA	C1-C2-C3	-2.59	121.56	126.04
31	C1	506	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	c1	511	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	R	612	CLA	CHA-C4D-ND	2.59	137.91	132.50
31	g	611	CLA	CHA-C4D-ND	2.59	137.91	132.50
31	N	602	CLA	C2C-C1C-NC	2.59	112.40	109.97
31	N	611	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	G1	613	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
56	R1	626	ERG	C14-C8-C7	-2.59	119.28	124.38
38	c1	524	DGA	OG1-CA1-CA2	2.59	120.03	111.91
31	n	614	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
47	n1	607	CHL	C2C-C3C-C4C	2.59	108.33	106.49
31	Y1	604	CLA	C1-C2-C3	-2.59	121.57	126.04
31	R	608	CLA	CMA-C3A-C4A	2.59	118.72	111.77
31	S1	604	CLA	C2D-C1D-ND	2.59	112.01	110.10
31	a1	410	CLA	C2D-C1D-ND	2.59	112.01	110.10
44	d1	405	PL9	C7-C8-C9	-2.58	122.49	126.79
31	C	513	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	b1	607	CLA	O2A-CGA-CBA	2.58	120.02	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	613	CLA	CMA-C3A-C4A	2.58	118.72	111.77
48	S1	621	LUT	C15-C14-C13	-2.58	123.62	127.31
31	y	611	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
31	R	608	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	s1	605	CLA	C1-O2A-CGA	2.58	123.22	116.44
31	C	508	CLA	CMA-C3A-C4A	2.58	118.71	111.77
47	S1	606	CHL	CMA-C3A-C4A	2.58	118.71	111.77
31	S1	611	CLA	CHA-C4D-ND	2.58	137.90	132.50
31	Y1	602	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
49	R	621	XAT	C31-C30-C29	-2.58	123.63	127.31
31	n1	610	CLA	C2D-C1D-ND	2.58	112.01	110.10
31	D	403	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	S1	604	CLA	O2A-CGA-CBA	2.58	120.01	111.91
31	g	604	CLA	CMA-C3A-C4A	2.58	118.71	111.77
48	s	620	LUT	C8-C7-C6	-2.58	119.96	127.20
31	B	613	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	y	611	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
47	n	606	CHL	CHB-C4A-NA	2.58	128.08	124.51
33	C1	516	BCR	C27-C26-C25	-2.58	118.99	122.73
31	S1	605	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
31	y1	603	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
47	g1	607	CHL	C1-C2-C3	-2.58	121.58	126.04
46	H1	101	RRX	C19-C18-C17	-2.58	114.98	118.94
49	R1	621	XAT	C18-C5-C6	-2.58	117.94	122.26
47	G	601	CHL	C1B-CHB-C4A	-2.58	125.01	130.12
31	R	602	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	S	614	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
31	B	613	CLA	CMA-C3A-C4A	2.58	118.70	111.77
31	R	612	CLA	O2A-CGA-CBA	2.58	120.00	111.91
57	Y1	626	PTY	O4-C30-C31	2.58	120.00	111.91
31	R	603	CLA	CHA-C4D-ND	2.58	137.89	132.50
31	G1	603	CLA	CHA-C4D-ND	2.58	137.89	132.50
31	Y	610	CLA	C2C-C1C-NC	2.58	112.39	109.97
31	y1	608	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
31	B1	608	CLA	CHA-C4D-ND	2.58	137.89	132.50
31	G1	614	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	c1	503	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
31	c1	510	CLA	CMB-C2B-C3B	2.58	129.50	124.68
31	g	604	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
47	S1	606	CHL	CHB-C4A-NA	2.58	128.07	124.51
31	Y1	608	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
31	R1	602	CLA	C2C-C1C-NC	2.58	112.39	109.97

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	501	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
52	s	626	3PH	O31-C31-C32	2.58	119.99	111.91
47	y1	601	CHL	C1-O2A-CGA	2.58	123.20	116.44
31	n1	611	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
50	r1	622	NEX	C38-C25-C26	-2.57	117.95	122.26
31	r	613	CLA	C2D-C1D-ND	2.57	112.00	110.10
31	R	609	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
31	A1	406	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
35	B	622	LMG	O8-C28-C29	2.57	119.98	111.91
31	s	609	CLA	C1-C2-C3	-2.57	121.59	126.04
37	B	620	C7Z	C22-C23-C24	2.57	113.83	110.30
31	r1	608	CLA	C2D-C1D-ND	2.57	112.00	110.10
31	s1	614	CLA	C2D-C1D-ND	2.57	112.00	110.10
31	B	606	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
31	R	611	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
47	N1	605	CHL	C4D-CHA-C1A	2.57	124.38	121.25
31	S	611	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
38	C1	524	DGA	OG1-CA1-CA2	2.57	119.98	111.91
31	y1	608	CLA	CHA-C4D-ND	2.57	137.88	132.50
31	B	608	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
31	r	603	CLA	C2D-C1D-ND	2.57	112.00	110.10
31	g1	611	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
31	S	611	CLA	CHA-C4D-ND	2.57	137.87	132.50
31	S	617	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
47	y1	606	CHL	C1-O2A-CGA	2.57	123.19	116.44
31	B1	610	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
41	D	409	LHG	O8-C23-C24	2.57	119.97	111.91
31	N1	612	CLA	CMA-C3A-C4A	2.57	118.68	111.77
31	C1	511	CLA	O2A-CGA-CBA	2.57	119.97	111.91
47	s1	607	CHL	CHB-C4A-NA	2.57	128.06	124.51
31	R1	612	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
31	b	606	CLA	O2A-CGA-CBA	2.57	119.97	111.91
31	b1	615	CLA	CHA-C4D-ND	2.57	137.87	132.50
48	y1	621	LUT	C40-C33-C34	-2.57	119.33	122.92
50	S	622	NEX	C40-C33-C34	-2.57	119.33	122.92
31	N1	610	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
44	d	405	PL9	C40-C39-C41	2.57	119.59	115.27
31	s	613	CLA	C2D-C1D-ND	2.57	112.00	110.10
33	c	517	BCR	C33-C5-C6	-2.57	121.64	124.53
31	Y1	603	CLA	OBD-CAD-C3D	-2.57	122.34	128.52
47	S1	608	CHL	C3C-C4C-NC	-2.57	107.69	110.57
47	N1	608	CHL	C4D-CHA-C1A	2.57	124.37	121.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	613	CLA	CMD-C2D-C3D	-2.57	121.71	127.61
31	y1	602	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
31	Y1	610	CLA	C2C-C1C-NC	2.57	112.38	109.97
31	y	614	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
31	c1	510	CLA	CHA-C4D-ND	2.57	137.87	132.50
47	S	608	CHL	C1-O2A-CGA	2.57	123.17	116.44
31	c1	513	CLA	CMA-C3A-C4A	2.57	118.67	111.77
31	n1	612	CLA	CMA-C3A-C4A	2.57	118.67	111.77
31	R	610	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
50	R1	622	NEX	C5-C4-C3	-2.56	108.71	111.75
31	A1	407	CLA	CMB-C2B-C3B	2.56	129.47	124.68
31	S1	610	CLA	C1-C2-C3	-2.56	121.61	126.04
31	r	603	CLA	CHA-C4D-ND	2.56	137.86	132.50
31	G	602	CLA	C1-C2-C3	-2.56	121.61	126.04
48	y1	621	LUT	C11-C10-C9	-2.56	123.65	127.31
47	S1	608	CHL	C4D-CHA-C1A	2.56	124.37	121.25
47	s	606	CHL	CHB-C4A-NA	2.56	128.06	124.51
31	B	616	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
31	B1	614	CLA	C1-C2-C3	-2.56	121.61	126.04
31	B	605	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
41	N1	624	LHG	C5-O7-C7	-2.56	111.48	117.79
31	b1	606	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
31	A	406	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	b	611	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
47	N1	608	CHL	C3A-C2A-C1A	2.56	105.18	101.34
35	A1	413	LMG	O8-C28-C29	2.56	119.95	111.91
47	g	609	CHL	C1-C2-C3	-2.56	121.61	126.04
31	b1	617	CLA	CHA-C4D-ND	2.56	137.86	132.50
50	S1	623	NEX	C38-C25-C26	-2.56	117.97	122.26
47	s	607	CHL	CHB-C4A-NA	2.56	128.05	124.51
47	g	606	CHL	C4D-CHA-C1A	2.56	124.36	121.25
31	c	507	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
47	g	607	CHL	C1-O2A-CGA	2.56	123.16	116.44
31	a	410	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
31	y	610	CLA	CMB-C2B-C3B	2.56	129.47	124.68
47	y1	609	CHL	C1-C2-C3	-2.56	121.62	126.04
31	R	609	CLA	O2A-CGA-CBA	2.56	119.94	111.91
31	d1	402	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
31	y1	604	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
31	S1	603	CLA	CHA-C4D-ND	2.56	137.85	132.50
31	r	609	CLA	O2A-CGA-CBA	2.56	119.93	111.91
31	c	511	CLA	C2C-C1C-NC	2.56	112.37	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	602	CLA	CMA-C3A-C4A	2.56	118.65	111.77
31	b	605	CLA	CHD-C1D-ND	-2.56	122.10	124.45
31	B1	615	CLA	CHA-C4D-ND	2.56	137.85	132.50
31	y1	612	CLA	CHA-C4D-ND	2.56	137.85	132.50
49	G	622	XAT	C19-C9-C10	-2.56	119.34	122.92
31	S1	609	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
47	y1	606	CHL	C2C-C3C-C4C	2.56	108.31	106.49
32	A1	408	PHO	O1D-CGD-CBD	2.56	129.00	124.74
31	y	612	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
37	B1	620	C7Z	C20-C13-C14	-2.56	119.34	122.92
47	y	601	CHL	C4D-CHA-C1A	2.56	124.36	121.25
44	D	405	PL9	C22-C23-C24	-2.56	121.51	127.66
31	C	501	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	N1	613	CLA	C2D-C1D-ND	2.56	111.99	110.10
48	n	621	LUT	C38-C25-C24	-2.56	118.09	123.56
31	N	610	CLA	CAA-CBA-CGA	2.55	120.72	113.25
47	n1	606	CHL	C1-O2A-CGA	2.55	123.15	116.44
31	n1	612	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
33	b	618	BCR	C33-C5-C6	-2.55	121.66	124.53
31	n	612	CLA	C4D-CHA-C1A	2.55	124.36	121.25
31	b1	606	CLA	CHA-C4D-ND	2.55	137.84	132.50
31	b	609	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
31	C	507	CLA	C2D-C1D-ND	2.55	111.98	110.10
31	y	612	CLA	C2D-C1D-ND	2.55	111.98	110.10
31	y	610	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
31	G	602	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
31	C1	502	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
31	y	610	CLA	O2A-CGA-CBA	2.55	119.92	111.91
41	D1	410	LHG	O8-C23-C24	2.55	119.92	111.91
31	G1	611	CLA	CMD-C2D-C3D	-2.55	121.74	127.61
31	c1	511	CLA	CMB-C2B-C3B	2.55	129.45	124.68
31	Y	613	CLA	O2A-CGA-CBA	2.55	119.92	111.91
33	a	411	BCR	C35-C13-C12	2.55	122.10	118.08
31	g	604	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
33	B	618	BCR	C33-C5-C4	2.55	118.52	113.62
33	C1	516	BCR	C33-C5-C4	2.55	118.52	113.62
31	y	613	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
49	y	622	XAT	C38-C25-C26	-2.55	117.99	122.26
31	S	609	CLA	C1-C2-C3	-2.55	121.63	126.04
31	s1	611	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
31	s	605	CLA	O2A-CGA-CBA	2.55	119.91	111.91
33	C1	516	BCR	C15-C14-C13	-2.55	123.67	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	608	CLA	C2D-C1D-ND	2.55	111.98	110.10
31	r1	612	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
50	r1	622	NEX	C40-C33-C34	-2.55	119.35	122.92
31	b	611	CLA	CMC-C2C-C1C	2.55	128.92	125.04
56	R1	626	ERG	C13-C14-C8	2.55	118.42	113.48
31	R	609	CLA	CHA-C4D-ND	2.55	137.83	132.50
31	D1	402	CLA	C1-C2-C3	-2.55	121.64	126.04
47	G1	607	CHL	C1-C2-C3	-2.55	121.64	126.04
31	b1	612	CLA	O2A-CGA-CBA	2.55	119.90	111.91
31	g1	604	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
31	n	612	CLA	CHA-C1A-NA	-2.55	120.56	126.40
31	c	501	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
49	Y1	622	XAT	C6-C7-C8	-2.55	120.61	125.99
31	d1	402	CLA	O2A-CGA-CBA	2.55	119.90	111.91
31	c	513	CLA	CMA-C3A-C4A	2.55	118.62	111.77
47	S1	607	CHL	C4D-CHA-C1A	2.55	124.35	121.25
31	G	614	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
47	s1	601	CHL	CHB-C4A-NA	2.55	128.03	124.51
33	c	516	BCR	C23-C22-C21	-2.55	115.03	118.94
31	A1	410	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
31	N1	602	CLA	CMB-C2B-C3B	2.55	129.44	124.68
31	g1	611	CLA	C2D-C1D-ND	2.55	111.98	110.10
31	g1	610	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
31	C1	510	CLA	CHA-C4D-ND	2.55	137.82	132.50
31	N1	613	CLA	CHA-C4D-ND	2.55	137.82	132.50
31	s	610	CLA	CMD-C2D-C3D	-2.54	121.76	127.61
31	Y	610	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
31	C	503	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	n	613	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	y	610	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
31	y	612	CLA	CHA-C4D-ND	2.54	137.82	132.50
31	G1	603	CLA	C2D-C1D-ND	2.54	111.98	110.10
31	C1	506	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
47	N1	607	CHL	C4A-NA-C1A	2.54	107.85	106.71
31	s1	605	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	B	604	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
31	a1	410	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
31	y	613	CLA	C2D-C1D-ND	2.54	111.98	110.10
31	a1	405	CLA	C2C-C1C-NC	2.54	112.35	109.97
31	r1	612	CLA	CHA-C4D-ND	2.54	137.81	132.50
31	r1	602	CLA	O2A-CGA-CBA	2.54	119.88	111.91
31	c	506	CLA	O2D-CGD-O1D	-2.54	118.87	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	603	CLA	C1D-ND-C4D	-2.54	104.53	106.33
31	b1	612	CLA	C1D-ND-C4D	-2.54	104.53	106.33
33	c1	514	BCR	C33-C5-C6	-2.54	121.67	124.53
31	B1	611	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
31	A1	405	CLA	CMD-C2D-C3D	-2.54	121.77	127.61
31	A	410	CLA	CHA-C4D-ND	2.54	137.81	132.50
41	D	410	LHG	O8-C23-C24	2.54	119.88	111.91
50	y	623	NEX	C1-C2-C3	2.54	119.38	113.64
31	n	604	CLA	CHA-C4D-ND	2.54	137.81	132.50
50	R	622	NEX	C16-C1-C6	-2.54	108.20	110.47
50	n	623	NEX	C31-C30-C29	2.54	130.93	127.31
31	C	506	CLA	CMA-C3A-C4A	2.54	118.59	111.77
31	r	604	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
47	S	608	CHL	C4A-NA-C1A	2.54	107.85	106.71
47	s1	601	CHL	C4A-NA-C1A	2.54	107.85	106.71
31	Y1	612	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
31	b1	615	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
52	s1	626	3PH	O31-C31-C32	2.54	119.87	111.91
31	B	615	CLA	CMD-C2D-C3D	-2.54	121.78	127.61
31	s	614	CLA	CHA-C4D-ND	2.54	137.81	132.50
31	N	604	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
31	c1	505	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
47	N1	609	CHL	C2C-C3C-C4C	2.54	108.30	106.49
31	N1	602	CLA	CMC-C2C-C1C	2.54	128.90	125.04
31	n1	613	CLA	C1-O2A-CGA	2.54	123.10	116.44
31	c	501	CLA	CHA-C4D-ND	2.54	137.80	132.50
31	g	604	CLA	CHA-C4D-ND	2.54	137.80	132.50
47	r1	607	CHL	CHB-C4A-NA	2.54	128.02	124.51
31	b1	604	CLA	C1D-ND-C4D	-2.54	104.53	106.33
41	G	630	LHG	O8-C23-C24	2.54	119.86	111.91
31	s	605	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	N1	602	CLA	O2A-CGA-CBA	2.53	119.86	111.91
50	G1	623	NEX	C4-C3-C2	2.53	115.67	110.77
53	Y1	625	SPH	C3-C4-C5	-2.53	119.14	124.79
31	C	507	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	C1	501	CLA	O2A-CGA-CBA	2.53	119.86	111.91
45	f	101	HEM	CHC-C4B-C3B	2.53	128.45	124.57
31	A	405	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	A	406	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
31	G	603	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
31	B	617	CLA	CHD-C1D-ND	-2.53	122.13	124.45
31	D1	402	CLA	C2C-C1C-NC	2.53	112.34	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A1	405	CLA	CMC-C2C-C3C	2.53	132.99	126.12
31	s	609	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
31	c	507	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	r	611	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	G1	604	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	N	602	CLA	O2A-CGA-CBA	2.53	119.85	111.91
31	C1	504	CLA	C2D-C1D-ND	2.53	111.97	110.10
31	B	606	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
47	G1	605	CHL	CHB-C4A-NA	2.53	128.01	124.51
31	c	510	CLA	C1D-ND-C4D	-2.53	104.54	106.33
31	s1	617	CLA	C1D-ND-C4D	-2.53	104.54	106.33
31	g	604	CLA	CMB-C2B-C3B	2.53	129.41	124.68
48	s1	621	LUT	C1-C6-C5	-2.53	119.05	122.61
31	c	511	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
31	B	602	CLA	CHA-C4D-ND	2.53	137.79	132.50
33	c1	516	BCR	C23-C24-C25	-2.53	120.10	127.20
46	H1	101	RRX	C30-C25-C26	-2.53	119.05	122.61
38	c	524	DGA	OG1-CA1-CA2	2.53	119.85	111.91
31	A	405	CLA	C2C-C1C-NC	2.53	112.34	109.97
31	G1	611	CLA	CHA-C4D-ND	2.53	137.79	132.50
31	c1	512	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
31	C1	505	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
31	b	607	CLA	C1-C2-C3	-2.53	121.67	126.04
48	s1	620	LUT	C38-C25-C24	-2.53	118.15	123.56
31	R	604	CLA	CHA-C4D-ND	2.53	137.79	132.50
31	s1	614	CLA	CHA-C4D-ND	2.53	137.79	132.50
31	C1	505	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
31	S	611	CLA	O2A-CGA-CBA	2.53	119.84	111.91
50	n	623	NEX	C17-C1-C6	-2.53	108.21	110.47
31	r1	603	CLA	O2A-CGA-CBA	2.53	119.84	111.91
47	y1	609	CHL	CHB-C4A-NA	2.53	128.01	124.51
31	B	604	CLA	O2A-CGA-CBA	2.53	119.84	111.91
31	y	614	CLA	C1-C2-C3	-2.53	121.67	126.04
31	S	609	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
47	N	605	CHL	C4D-CHA-C1A	2.53	124.33	121.25
48	N	620	LUT	C38-C25-C24	-2.53	118.15	123.56
47	G	608	CHL	CHB-C4A-NA	2.53	128.01	124.51
47	y	609	CHL	CHB-C4A-NA	2.53	128.01	124.51
31	R1	603	CLA	CHA-C4D-ND	2.53	137.79	132.50
48	R1	620	LUT	C35-C15-C14	-2.53	118.30	123.47
31	N	602	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
49	n	622	XAT	C20-C13-C14	-2.53	119.38	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	610	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
31	R1	609	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
31	C	511	CLA	CHA-C4D-ND	2.53	137.78	132.50
47	n1	609	CHL	C4D-CHA-C1A	2.53	124.32	121.25
31	R1	604	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
31	B	609	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
47	N	606	CHL	C1-O2A-CGA	2.53	123.07	116.44
31	r	612	CLA	CHA-C4D-ND	2.53	137.78	132.50
31	C	501	CLA	C1D-ND-C4D	-2.53	104.54	106.33
31	a	405	CLA	C1D-ND-C4D	-2.53	104.54	106.33
31	s	614	CLA	C2D-C1D-ND	2.53	111.97	110.10
31	r1	612	CLA	C2D-C1D-ND	2.53	111.97	110.10
31	y	604	CLA	O2A-CGA-CBA	2.52	119.83	111.91
31	g1	613	CLA	O2A-CGA-CBA	2.52	119.83	111.91
31	g	604	CLA	OBD-CAD-C3D	-2.52	122.44	128.52
33	c	514	BCR	C38-C26-C27	2.52	118.47	113.62
31	a1	405	CLA	CHA-C4D-ND	2.52	137.78	132.50
31	n1	604	CLA	CHA-C4D-ND	2.52	137.78	132.50
31	Y	603	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
31	s	603	CLA	CMA-C3A-C4A	2.52	118.56	111.77
47	N1	608	CHL	CHB-C4A-NA	2.52	128.00	124.51
47	G1	601	CHL	CMA-C3A-C4A	2.52	118.55	111.77
31	c1	513	CLA	CHA-C4D-ND	2.52	137.78	132.50
31	S	609	CLA	C2D-C1D-ND	2.52	111.96	110.10
31	S1	613	CLA	C2D-C1D-ND	2.52	111.96	110.10
31	Y1	613	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	r	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
31	Y	613	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
31	G1	604	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
31	C1	501	CLA	C2D-C1D-ND	2.52	111.96	110.10
49	n	622	XAT	C18-C5-C6	-2.52	118.04	122.26
31	y	608	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	S	603	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	Y1	614	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	y	603	CLA	C1-C2-C3	-2.52	121.69	126.04
47	Y	605	CHL	CHB-C4A-NA	2.52	127.99	124.51
31	c1	506	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	s	604	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
49	r1	621	XAT	C18-C5-C6	-2.52	118.04	122.26
31	b	604	CLA	CHA-C4D-ND	2.52	137.76	132.50
31	c1	501	CLA	O2A-CGA-CBA	2.52	119.81	111.91
50	n1	623	NEX	C40-C33-C34	-2.52	119.40	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	611	CLA	CHA-C4D-ND	2.52	137.76	132.50
33	c	516	BCR	C8-C9-C10	2.52	122.80	118.94
31	n	602	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
31	s	613	CLA	O1D-CGD-CBD	-2.52	119.34	124.48
31	b	608	CLA	CHA-C4D-ND	2.52	137.76	132.50
31	N1	610	CLA	C1-C2-C3	-2.52	121.69	126.04
50	s	623	NEX	C39-C29-C30	-2.51	119.40	122.92
31	y1	610	CLA	O2A-CGA-CBA	2.51	119.80	111.91
31	g1	614	CLA	CHA-C4D-ND	2.51	137.76	132.50
31	y1	612	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
31	B	608	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
31	n	614	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
31	C	505	CLA	CHA-C4D-ND	2.51	137.76	132.50
47	n1	601	CHL	C4A-NA-C1A	2.51	107.84	106.71
31	B	607	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
33	b	619	BCR	C4-C5-C6	-2.51	119.08	122.73
31	g	613	CLA	CHA-C4D-ND	2.51	137.75	132.50
33	c	514	BCR	C8-C9-C10	2.51	122.80	118.94
31	y	614	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	A	410	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
31	C1	513	CLA	CBA-CAA-C2A	2.51	121.28	113.86
32	a1	408	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
31	R	603	CLA	C2D-C1D-ND	2.51	111.95	110.10
31	R	608	CLA	CHA-C4D-ND	2.51	137.75	132.50
47	N	609	CHL	CHB-C4A-NA	2.51	127.98	124.51
31	C	505	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
48	y1	621	LUT	C38-C25-C24	-2.51	118.19	123.56
31	n	611	CLA	CHA-C4D-ND	2.51	137.75	132.50
33	c1	516	BCR	C35-C13-C14	-2.51	119.41	122.92
50	s	623	NEX	C40-C33-C34	-2.51	119.41	122.92
31	b	614	CLA	CHA-C4D-ND	2.51	137.75	132.50
40	c	520	DGD	O1G-C1A-C2A	2.51	119.79	111.91
31	B	610	CLA	CHD-C1D-ND	-2.51	122.15	124.45
31	b1	610	CLA	CHD-C1D-ND	-2.51	122.15	124.45
47	G1	609	CHL	C4D-CHA-C1A	2.51	124.30	121.25
31	s	603	CLA	C1-C2-C3	-2.51	121.70	126.04
31	G1	611	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
31	Y1	610	CLA	O2A-CGA-CBA	2.51	119.78	111.91
31	c	502	CLA	CMB-C2B-C3B	2.51	129.37	124.68
31	r1	608	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	R	608	CLA	C2D-C1D-ND	2.51	111.95	110.10
33	C1	517	BCR	C3-C4-C5	-2.51	109.60	114.08

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	613	CLA	CHA-C4D-ND	2.51	137.75	132.50
41	N1	624	LHG	O8-C23-C24	2.51	119.78	111.91
31	Y	614	CLA	CHA-C4D-ND	2.51	137.74	132.50
47	y1	606	CHL	C1B-CHB-C4A	-2.51	125.15	130.12
47	G1	608	CHL	C4A-NA-C1A	2.51	107.83	106.71
31	N1	611	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
31	B1	605	CLA	CMA-C3A-C4A	2.51	118.51	111.77
47	N1	601	CHL	CHB-C4A-NA	2.51	127.98	124.51
31	r	610	CLA	CHA-C4D-ND	2.51	137.74	132.50
47	y	605	CHL	C1B-CHB-C4A	-2.51	125.15	130.12
31	G1	612	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
48	R	620	LUT	C18-C5-C6	-2.51	121.71	124.53
45	f	101	HEM	C4B-CHC-C1C	2.51	125.86	122.56
31	C1	503	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
46	h	101	RRX	C24-C23-C22	-2.51	122.45	126.23
31	a	406	CLA	CHA-C4D-ND	2.51	137.74	132.50
31	R	612	CLA	CMD-C2D-C3D	-2.51	121.85	127.61
31	g	613	CLA	O2A-CGA-CBA	2.51	119.77	111.91
47	Y1	601	CHL	CHB-C4A-NA	2.51	127.98	124.51
47	n	609	CHL	C3C-C4C-NC	-2.50	107.76	110.57
31	Y1	611	CLA	C1C-C2C-C3C	-2.50	104.32	106.96
31	a1	410	CLA	CHA-C4D-ND	2.50	137.74	132.50
31	s	604	CLA	O2A-CGA-CBA	2.50	119.77	111.91
31	G	604	CLA	CHA-C4D-ND	2.50	137.74	132.50
31	r1	603	CLA	CHA-C4D-ND	2.50	137.74	132.50
31	s	604	CLA	CMA-C3A-C4A	2.50	118.50	111.77
31	r1	609	CLA	C2D-C1D-ND	2.50	111.95	110.10
49	R1	621	XAT	C26-C27-C28	-2.50	120.70	125.99
31	b	616	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
31	S1	611	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
31	n1	603	CLA	CHA-C4D-ND	2.50	137.74	132.50
31	C	506	CLA	CMB-C2B-C3B	2.50	129.36	124.68
33	c	516	BCR	C36-C18-C17	-2.50	119.42	122.92
31	c	501	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	S	610	CLA	O2A-CGA-CBA	2.50	119.76	111.91
47	n	608	CHL	C2C-C3C-C4C	2.50	108.27	106.49
31	B	604	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
31	C1	501	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	C	510	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
31	C1	507	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
50	y	623	NEX	C4-C3-C2	2.50	115.61	110.77
31	b1	608	CLA	C1-C2-C3	-2.50	121.72	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	614	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
47	g1	606	CHL	CHB-C4A-NA	2.50	127.97	124.51
47	R1	607	CHL	C4D-CHA-C1A	2.50	124.29	121.25
31	Y	612	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
31	g	603	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
31	g1	604	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
31	C1	507	CLA	C1-C2-C3	-2.50	121.72	126.04
56	r1	626	ERG	C13-C14-C8	2.50	118.33	113.48
31	B	616	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	B1	604	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	b	602	CLA	CHA-C4D-ND	2.50	137.73	132.50
33	b1	618	BCR	C23-C24-C25	-2.50	120.18	127.20
47	G1	601	CHL	C1-O2A-CGA	2.50	123.00	116.44
31	b	606	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	R1	612	CLA	CHA-C4D-ND	2.50	137.73	132.50
41	C	525	LHG	O8-C23-C24	2.50	119.75	111.91
37	b1	620	C7Z	C20-C13-C14	-2.50	119.42	122.92
49	g1	622	XAT	C19-C9-C10	-2.50	119.42	122.92
31	N	603	CLA	C2D-C1D-ND	2.50	111.94	110.10
31	B1	610	CLA	O2A-CGA-CBA	2.50	119.75	111.91
54	K1	101	4RF	O40-C41-C43	2.50	119.75	111.91
31	d1	402	CLA	CMA-C3A-C4A	2.50	118.49	111.77
48	S1	621	LUT	C18-C5-C4	2.50	118.98	114.36
31	a	405	CLA	CMA-C3A-C4A	2.50	118.48	111.77
31	B	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	S1	605	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	B1	611	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	B	607	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
31	C1	512	CLA	CMB-C2B-C1B	-2.50	124.63	128.46
31	C1	513	CLA	C2C-C1C-NC	2.50	112.31	109.97
31	A	405	CLA	CMD-C2D-C3D	-2.50	121.87	127.61
33	C	517	BCR	C36-C18-C17	-2.50	119.43	122.92
31	N	604	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	c	502	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	n	613	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	n1	610	CLA	O2A-CGA-CBA	2.50	119.74	111.91
31	G	614	CLA	CMB-C2B-C3B	2.50	129.35	124.68
47	r1	607	CHL	CHD-C4C-C3C	2.50	128.51	124.84
31	Y1	611	CLA	CHA-C4D-ND	2.50	137.72	132.50
56	R1	626	ERG	C1-C10-C5	2.49	113.32	108.75
31	R1	610	CLA	C1D-ND-C4D	-2.49	104.56	106.33
31	a	406	CLA	CMD-C2D-C3D	-2.49	121.88	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B1	618	BCR	C37-C22-C21	-2.49	119.43	122.92
31	s	612	CLA	C1C-C2C-C3C	-2.49	104.33	106.96
31	S1	609	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
31	s1	613	CLA	CHA-C4D-ND	2.49	137.72	132.50
50	y	623	NEX	C11-C10-C9	2.49	130.87	127.31
31	s	611	CLA	O2A-CGA-CBA	2.49	119.73	111.91
31	s1	602	CLA	C2C-C1C-NC	2.49	112.31	109.97
31	S	609	CLA	CHA-C4D-ND	2.49	137.72	132.50
31	y1	614	CLA	CHA-C4D-ND	2.49	137.72	132.50
31	Y	608	CLA	C1C-C2C-C3C	-2.49	104.33	106.96
31	C	512	CLA	C1-C2-C3	-2.49	121.73	126.04
31	C	510	CLA	O2A-CGA-CBA	2.49	119.73	111.91
47	s	601	CHL	CHB-C4A-NA	2.49	127.96	124.51
31	c	502	CLA	CMC-C2C-C1C	2.49	128.84	125.04
48	N	621	LUT	C35-C15-C14	-2.49	118.37	123.47
49	r1	621	XAT	C25-C24-C23	-2.49	107.82	112.75
31	r	612	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
47	y	601	CHL	C1B-CHB-C4A	-2.49	125.18	130.12
31	N1	610	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	N1	612	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	y	612	CLA	CHD-C1D-ND	-2.49	122.17	124.45
31	y	612	CLA	O2A-CGA-CBA	2.49	119.72	111.91
33	c1	517	BCR	C34-C9-C10	-2.49	119.43	122.92
47	S1	607	CHL	C1B-CHB-C4A	-2.49	125.18	130.12
31	y	604	CLA	CHA-C4D-ND	2.49	137.71	132.50
37	b1	620	C7Z	C38-C25-C24	2.49	118.97	114.36
48	y1	621	LUT	C35-C15-C14	-2.49	118.37	123.47
54	I1	102	4RF	O18-C16-C15	2.49	119.72	111.91
31	r	611	CLA	C2D-C1D-ND	2.49	111.94	110.10
31	y	608	CLA	C2D-C1D-ND	2.49	111.94	110.10
31	y	608	CLA	C1-O2A-CGA	2.49	122.98	116.44
50	N1	623	NEX	C20-C13-C14	-2.49	119.44	122.92
31	B	602	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
33	B	619	BCR	C4-C5-C6	-2.49	119.12	122.73
31	g1	612	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	s	602	CLA	C1D-ND-C4D	-2.49	104.57	106.33
31	R1	604	CLA	CHA-C4D-ND	2.49	137.71	132.50
33	b	618	BCR	C36-C18-C17	-2.49	119.44	122.92
31	B1	604	CLA	O2A-CGA-CBA	2.49	119.72	111.91
31	r1	612	CLA	CHA-C1A-NA	-2.49	120.70	126.40
31	C	501	CLA	O2A-CGA-CBA	2.49	119.72	111.91
31	N	613	CLA	CHA-C4D-ND	2.49	137.70	132.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	511	CLA	O2A-CGA-CBA	2.49	119.71	111.91
31	c	513	CLA	CHD-C1D-ND	-2.49	122.17	124.45
31	N1	613	CLA	CHD-C1D-ND	-2.49	122.17	124.45
31	Y1	611	CLA	C2D-C1D-ND	2.49	111.94	110.10
31	B1	604	CLA	C2C-C1C-NC	2.49	112.30	109.97
48	y	620	LUT	C39-C29-C28	2.49	122.00	118.08
55	R1	625	LMT	C3'-C4'-C5'	-2.49	105.22	110.93
31	C	506	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
31	r	610	CLA	O2A-CGA-CBA	2.49	119.71	111.91
31	N1	611	CLA	CHA-C4D-ND	2.49	137.70	132.50
48	n	620	LUT	C35-C15-C14	-2.49	118.38	123.47
50	g	623	NEX	C4-C3-C2	2.49	115.57	110.77
31	C	511	CLA	CMB-C2B-C3B	2.49	129.33	124.68
50	s	623	NEX	C20-C13-C14	-2.49	119.44	122.92
31	D	403	CLA	O2A-CGA-CBA	2.48	119.71	111.91
31	b1	602	CLA	CHA-C4D-ND	2.48	137.70	132.50
31	b	613	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
31	c	504	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
31	b1	605	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
31	r1	602	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
31	r	602	CLA	CMA-C3A-C4A	2.48	118.45	111.77
31	b	610	CLA	C2D-C1D-ND	2.48	111.94	110.10
33	c1	514	BCR	C40-C30-C25	-2.48	106.27	110.30
31	S	604	CLA	CMA-C3A-C4A	2.48	118.45	111.77
31	N	602	CLA	CAA-C2A-C3A	-2.48	105.97	112.78
31	Y	604	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
31	G	603	CLA	C1-C2-C3	-2.48	121.75	126.04
31	b1	614	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	N	612	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	Y1	610	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
31	S1	609	CLA	C1D-ND-C4D	-2.48	104.57	106.33
31	Y	604	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	r	602	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
47	n	606	CHL	C1-O2A-CGA	2.48	122.96	116.44
31	n1	610	CLA	C1-C2-C3	-2.48	121.75	126.04
47	g	601	CHL	CHB-C4A-NA	2.48	127.94	124.51
47	S1	607	CHL	CHB-C4A-NA	2.48	127.94	124.51
31	c1	507	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
31	c1	511	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	D1	403	CLA	C2D-C1D-ND	2.48	111.93	110.10
31	n1	602	CLA	O2A-CGA-CBA	2.48	119.70	111.91
31	d1	403	CLA	CMA-C3A-C2A	2.48	123.84	113.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y1	603	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
31	C1	505	CLA	CMB-C2B-C3B	2.48	129.32	124.68
31	B1	614	CLA	CHA-C4D-ND	2.48	137.69	132.50
37	B	620	C7Z	C20-C13-C14	-2.48	119.45	122.92
49	G	622	XAT	C40-C33-C34	-2.48	119.45	122.92
31	c1	505	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
31	y	612	CLA	C1-C2-C3	-2.48	121.75	126.04
50	R1	622	NEX	C38-C25-C26	-2.48	118.10	122.26
31	b	605	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	B1	607	CLA	CMD-C2D-C3D	-2.48	121.91	127.61
33	B	619	BCR	C28-C27-C26	-2.48	109.65	114.08
31	b1	607	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
31	c1	504	CLA	C1-O2A-CGA	2.48	122.95	116.44
31	S1	610	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	y	611	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	s	604	CLA	C2D-C1D-ND	2.48	111.93	110.10
33	b1	618	BCR	C4-C5-C6	-2.48	119.13	122.73
31	C	506	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
31	R	603	CLA	C1-C2-C3	-2.48	121.76	126.04
31	c	501	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
31	S	604	CLA	O2A-CGA-CBA	2.48	119.68	111.91
56	R1	626	ERG	C19-C10-C1	-2.48	105.52	109.43
47	Y	601	CHL	C1-C2-C3	-2.48	121.76	126.04
31	B	603	CLA	CMA-C3A-C4A	2.48	118.43	111.77
31	S1	604	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	c	506	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
31	C1	509	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
47	N	605	CHL	C1B-CHB-C4A	-2.48	125.21	130.12
49	R	621	XAT	C11-C10-C9	-2.48	123.78	127.31
31	C	507	CLA	CHA-C1A-NA	-2.48	120.73	126.40
31	B	608	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	C1	509	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	y1	612	CLA	O2A-CGA-CBA	2.48	119.68	111.91
47	N1	607	CHL	C4D-CHA-C1A	2.48	124.26	121.25
31	g	612	CLA	CHA-C4D-ND	2.48	137.68	132.50
47	N1	605	CHL	C1-C2-C3	-2.48	121.76	126.04
33	c1	515	BCR	C36-C18-C17	-2.48	119.46	122.92
31	C1	505	CLA	O2A-CGA-CBA	2.47	119.67	111.91
31	B	610	CLA	CHA-C4D-ND	2.47	137.68	132.50
31	B1	605	CLA	CHA-C4D-ND	2.47	137.68	132.50
31	Y1	610	CLA	CMA-C3A-C4A	2.47	118.42	111.77
31	B	604	CLA	CHD-C1D-ND	-2.47	122.18	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	S1	624	LHG	O8-C23-C24	2.47	119.67	111.91
48	S	620	LUT	C11-C10-C9	-2.47	123.78	127.31
31	c	509	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
48	s1	620	LUT	C39-C29-C28	2.47	121.97	118.08
47	N	601	CHL	CHB-C4A-NA	2.47	127.93	124.51
31	C1	506	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	c1	502	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	Y	603	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	c	509	CLA	CMD-C2D-C3D	-2.47	121.92	127.61
48	R	620	LUT	C19-C9-C10	-2.47	119.46	122.92
49	Y	622	XAT	C26-C27-C28	-2.47	120.77	125.99
31	G1	610	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
56	R1	626	ERG	C18-C13-C14	-2.47	106.24	110.24
31	R	603	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
31	B1	606	CLA	C1-O2A-CGA	2.47	122.93	116.44
49	y	622	XAT	O24-C25-C38	-2.47	112.09	115.06
31	S	610	CLA	CMA-C3A-C4A	2.47	118.42	111.77
31	N	612	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
31	c1	502	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
31	A	410	CLA	O2A-CGA-CBA	2.47	119.67	111.91
31	C1	501	CLA	C1D-ND-C4D	-2.47	104.58	106.33
47	r	606	CHL	CHB-C4A-NA	2.47	127.93	124.51
31	b1	616	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	N	612	CLA	CHD-C1D-ND	-2.47	122.18	124.45
31	b	617	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
31	g1	612	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
31	b1	608	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
47	G1	608	CHL	C1B-CHB-C4A	-2.47	125.22	130.12
31	y1	610	CLA	CMB-C2B-C3B	2.47	129.30	124.68
31	Y	608	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	n1	613	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	b1	604	CLA	O2A-CGA-CBA	2.47	119.66	111.91
31	G	604	CLA	C2D-C1D-ND	2.47	111.92	110.10
31	Y	614	CLA	C2D-C1D-ND	2.47	111.92	110.10
31	S	612	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
31	Y1	604	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
31	S1	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	b	615	CLA	C1-O2A-CGA	2.47	122.92	116.44
47	g	601	CHL	C1B-CHB-C4A	-2.47	125.23	130.12
31	N	603	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
48	N	620	LUT	C31-C32-C33	-2.47	119.48	126.42
31	b	615	CLA	CMD-C2D-C3D	-2.47	121.94	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	608	CLA	CMB-C2B-C3B	2.47	129.30	124.68
31	B1	617	CLA	CHA-C4D-ND	2.47	137.66	132.50
33	C1	514	BCR	C23-C24-C25	-2.47	120.27	127.20
31	n	602	CLA	O2A-CGA-CBA	2.47	119.65	111.91
31	S1	614	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	S1	612	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
31	c	512	CLA	O2A-CGA-CBA	2.47	119.65	111.91
47	g1	608	CHL	C3C-C4C-NC	-2.47	107.80	110.57
31	G	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	G1	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	y1	613	CLA	CHA-C4D-ND	2.47	137.66	132.50
41	Y1	624	LHG	O8-C23-C24	2.47	119.65	111.91
31	C	510	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	g	613	CLA	C1-C2-C3	-2.47	121.78	126.04
47	N1	607	CHL	CHB-C4A-NA	2.47	127.92	124.51
31	a	407	CLA	CHA-C4D-ND	2.47	137.66	132.50
32	A	408	PHO	O1D-CGD-CBD	2.47	128.84	124.74
47	g	605	CHL	CHB-C4A-NA	2.47	127.92	124.51
31	B	603	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	C1	504	CLA	CMD-C2D-C3D	-2.47	121.94	127.61
45	F1	101	HEM	C4B-CHC-C1C	2.46	125.81	122.56
31	N	611	CLA	O1D-CGD-CBD	-2.46	119.44	124.48
47	n1	605	CHL	C4A-NA-C1A	2.46	107.81	106.71
31	c1	507	CLA	CMB-C2B-C3B	2.46	129.29	124.68
47	g	607	CHL	C1B-CHB-C4A	-2.46	125.24	130.12
31	r	604	CLA	CHA-C4D-ND	2.46	137.65	132.50
46	h	101	RRX	C23-C24-C25	-2.46	120.28	127.20
31	Y1	614	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
31	s1	613	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
47	G1	608	CHL	CHB-C4A-NA	2.46	127.92	124.51
31	G	612	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
31	D1	403	CLA	CHA-C4D-ND	2.46	137.65	132.50
48	s	620	LUT	C11-C12-C13	-2.46	119.50	126.42
37	B	620	C7Z	C21-C26-C25	-2.46	119.14	122.61
47	S	607	CHL	CHB-C4A-NA	2.46	127.92	124.51
50	R	622	NEX	C39-C29-C30	-2.46	119.47	122.92
47	s	606	CHL	C1B-CHB-C4A	-2.46	125.24	130.12
31	s1	614	CLA	CHD-C1D-ND	-2.46	122.19	124.45
31	g	610	CLA	O2A-CGA-CBA	2.46	119.64	111.91
38	B1	625	DGA	OG1-CA1-CA2	2.46	119.64	111.91
31	s1	611	CLA	CHA-C1A-NA	-2.46	120.76	126.40
47	S	607	CHL	C4A-NA-C1A	2.46	107.81	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C	514	BCR	C33-C5-C6	-2.46	121.76	124.53
31	Y1	602	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
31	Y	610	CLA	CHA-C4D-ND	2.46	137.65	132.50
31	B1	610	CLA	CHA-C4D-ND	2.46	137.65	132.50
40	C1	518	DGD	O1G-C1A-C2A	2.46	119.63	111.91
31	b	602	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
31	c1	513	CLA	CMB-C2B-C3B	2.46	129.28	124.68
31	B1	605	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
31	S	613	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
31	N1	603	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
31	B	611	CLA	C1D-ND-C4D	-2.46	104.59	106.33
31	Y	603	CLA	C1D-ND-C4D	-2.46	104.59	106.33
31	G1	614	CLA	CHA-C4D-ND	2.46	137.65	132.50
31	C1	511	CLA	C2D-C1D-ND	2.46	111.92	110.10
31	y1	612	CLA	C2D-C1D-ND	2.46	111.92	110.10
31	n1	613	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
50	s	623	NEX	C1-C2-C3	2.46	119.20	113.64
31	b1	606	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
31	g	614	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	r1	609	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
40	c1	519	DGD	O1G-C1A-O1A	-2.46	117.39	123.59
31	N	604	CLA	C2C-C1C-NC	2.46	112.28	109.97
31	b	614	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
31	y	614	CLA	O2A-CGA-CBA	2.46	119.62	111.91
31	r	611	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
31	n	603	CLA	CHA-C4D-ND	2.46	137.64	132.50
37	B	620	C7Z	C28-C27-C26	-2.46	120.30	127.20
31	D	403	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
31	g	602	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
31	S1	609	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	S	617	CLA	O2A-CGA-CBA	2.46	119.62	111.91
31	S	610	CLA	CHD-C1D-ND	-2.46	122.19	124.45
31	b	610	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	S1	614	CLA	O2A-CGA-CBA	2.46	119.62	111.91
31	y	613	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	Y1	604	CLA	CMB-C2B-C3B	2.46	129.28	124.68
49	G	622	XAT	C18-C5-C6	-2.46	118.14	122.26
31	s1	602	CLA	CMA-C3A-C4A	2.46	118.38	111.77
31	s	612	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	A1	406	CLA	C1D-ND-C4D	-2.46	104.59	106.33
31	R	611	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	g1	602	CLA	CMC-C2C-C1C	2.46	128.78	125.04

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	504	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	s1	602	CLA	CMB-C2B-C3B	2.46	129.27	124.68
47	n1	605	CHL	C1B-CHB-C4A	-2.46	125.25	130.12
31	R1	604	CLA	CMD-C2D-C3D	-2.46	121.97	127.61
31	r1	603	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
31	b1	614	CLA	C1-C2-C3	-2.46	121.80	126.04
31	c	510	CLA	O2A-CGA-CBA	2.45	119.61	111.91
31	R	613	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	Y	613	CLA	CHA-C4D-ND	2.45	137.63	132.50
33	B	618	BCR	C37-C22-C23	2.45	121.94	118.08
48	r1	620	LUT	C8-C7-C6	-2.45	120.31	127.20
31	B1	616	CLA	CHA-C4D-ND	2.45	137.63	132.50
49	y	622	XAT	C6-C7-C8	-2.45	120.81	125.99
31	s	611	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	R1	608	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
31	R1	602	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	s1	610	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	s	614	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
31	C	503	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	y	613	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
31	g1	610	CLA	CMD-C2D-C3D	-2.45	121.97	127.61
31	a	410	CLA	CHA-C4D-ND	2.45	137.63	132.50
47	g1	601	CHL	C4A-NA-C1A	2.45	107.81	106.71
31	y1	603	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
31	G	602	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	c	502	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	d1	402	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	c1	505	CLA	CHD-C1D-ND	-2.45	122.20	124.45
47	y	609	CHL	C1-O2A-CGA	2.45	122.87	116.44
31	G	602	CLA	CMB-C2B-C3B	2.45	129.26	124.68
31	C	505	CLA	C2D-C1D-ND	2.45	111.91	110.10
31	a	407	CLA	C2D-C1D-ND	2.45	111.91	110.10
41	D1	410	LHG	C5-O7-C7	-2.45	111.76	117.79
31	s1	602	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	Y	602	CLA	C2C-C1C-NC	2.45	112.27	109.97
31	y1	604	CLA	CMA-C3A-C4A	2.45	118.35	111.77
47	G1	601	CHL	CHD-C4C-C3C	2.45	128.44	124.84
48	n1	621	LUT	C3-C4-C5	-2.45	106.98	111.85
31	N	614	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
33	a1	411	BCR	C34-C9-C10	-2.45	119.49	122.92
31	d	402	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	b1	605	CLA	CHA-C4D-ND	2.45	137.62	132.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d1	403	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	g1	611	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	N1	604	CLA	O2A-CGA-CBA	2.45	119.59	111.91
31	B	611	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
31	Y1	603	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	Y1	610	CLA	CAA-C2A-C3A	-2.45	106.08	112.78
31	R1	603	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
31	B	605	CLA	CMD-C2D-C3D	-2.45	121.99	127.61
33	A	411	BCR	C35-C13-C12	2.45	121.93	118.08
31	n1	612	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
48	g	621	LUT	C38-C25-C24	-2.45	118.33	123.56
31	D1	403	CLA	CMA-C3A-C4A	2.45	118.34	111.77
31	C	509	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
47	G1	609	CHL	CHB-C4A-NA	2.44	127.89	124.51
31	g1	602	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	S1	603	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
31	s1	614	CLA	O2A-CGA-CBA	2.44	119.58	111.91
31	N1	602	CLA	C2C-C1C-NC	2.44	112.26	109.97
31	b	606	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
41	l	101	LHG	O8-C23-C24	2.44	119.58	111.91
31	C1	507	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
31	r1	603	CLA	C2D-C1D-ND	2.44	111.91	110.10
31	C1	507	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	y	603	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	B	616	CLA	CHA-C1A-NA	-2.44	120.80	126.40
31	R1	608	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	a	407	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
31	B	605	CLA	CMA-C3A-C4A	2.44	118.34	111.77
47	y	606	CHL	CHB-C4A-NA	2.44	127.89	124.51
47	s1	606	CHL	CHB-C4A-NA	2.44	127.89	124.51
31	C1	501	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
31	S	617	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	R	612	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
33	c1	515	BCR	C1-C6-C7	2.44	122.69	115.78
31	c	501	CLA	C2D-C1D-ND	2.44	111.90	110.10
48	Y	620	LUT	C7-C8-C9	-2.44	122.55	126.23
31	A1	407	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
31	r1	609	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
31	C	511	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
31	C1	503	CLA	C2D-C1D-ND	2.44	111.90	110.10
33	d	404	BCR	C23-C24-C25	-2.44	120.35	127.20
44	d	405	PL9	C22-C23-C24	-2.44	121.79	127.66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	R1	626	ERG	C6-C7-C8	-2.44	117.27	122.07
31	B1	607	CLA	C1-C2-C3	-2.44	121.83	126.04
31	C1	503	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
47	n	609	CHL	CHB-C4A-NA	2.44	127.88	124.51
47	Y	605	CHL	C1B-CHB-C4A	-2.44	125.29	130.12
31	S	605	CLA	CHA-C4D-ND	2.44	137.60	132.50
47	N1	605	CHL	CHB-C4A-NA	2.44	127.88	124.51
31	A	407	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	b	607	CLA	O2A-CGA-CBA	2.44	119.56	111.91
35	c	521	LMG	O8-C28-C29	2.44	119.56	111.91
33	C	515	BCR	C35-C13-C12	2.44	121.92	118.08
47	G	606	CHL	C1-O2A-CGA	2.44	122.84	116.44
31	S	612	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	R1	612	CLA	CMA-C3A-C4A	2.44	118.32	111.77
40	B1	623	DGD	O5D-C6D-C5D	2.44	113.56	109.05
31	s1	611	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
41	y	624	LHG	O8-C23-C24	2.44	119.55	111.91
31	D1	402	CLA	O2A-CGA-CBA	2.44	119.55	111.91
31	c1	510	CLA	C2D-C1D-ND	2.44	111.90	110.10
31	Y1	602	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
31	N1	603	CLA	CMA-C3A-C4A	2.44	118.32	111.77
31	B	614	CLA	C1D-ND-C4D	-2.44	104.61	106.33
31	a1	406	CLA	C1D-ND-C4D	-2.44	104.61	106.33
31	b	608	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
47	g	608	CHL	CHB-C4A-NA	2.43	127.88	124.51
40	C	518	DGD	O6D-C5D-C6D	2.43	111.58	106.67
31	s	609	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
31	Y1	611	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
31	A1	410	CLA	CMC-C2C-C1C	2.43	128.75	125.04
33	c	515	BCR	C29-C30-C25	-2.43	106.73	110.48
31	C	510	CLA	C1D-ND-C4D	-2.43	104.61	106.33
48	n1	620	LUT	C22-C23-C24	-2.43	108.97	111.74
50	n	623	NEX	C16-C1-C6	-2.43	108.29	110.47
31	d	403	CLA	C2D-C1D-ND	2.43	111.90	110.10
47	N1	601	CHL	C1-O2A-CGA	2.43	122.83	116.44
31	N1	604	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
31	y1	602	CLA	C1D-ND-C4D	-2.43	104.61	106.33
31	c	503	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
33	C1	514	BCR	C38-C26-C25	-2.43	121.80	124.53
41	d	408	LHG	C6-C5-C4	-2.43	106.04	111.79
31	G	613	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
31	G	610	CLA	C3D-C2D-C1D	-2.43	102.51	105.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	N	607	CHL	C1-O2A-CGA	2.43	122.82	116.44
31	d	403	CLA	CHA-C4D-ND	2.43	137.59	132.50
47	g	607	CHL	C4D-CHA-C1A	2.43	124.21	121.25
31	c1	512	CLA	C1-O2A-CGA	2.43	122.82	116.44
31	S	609	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
37	B1	620	C7Z	C1-C6-C7	2.43	122.65	115.78
31	y	604	CLA	C2D-C1D-ND	2.43	111.89	110.10
31	N1	611	CLA	C2D-C1D-ND	2.43	111.89	110.10
31	b1	609	CLA	CHA-C1A-NA	-2.43	120.83	126.40
48	s1	620	LUT	C35-C15-C14	-2.43	118.50	123.47
33	b1	618	BCR	C34-C9-C10	-2.43	119.52	122.92
31	c	503	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	C1	513	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	C1	512	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	y1	602	CLA	CHA-C4D-ND	2.43	137.58	132.50
33	c	517	BCR	C33-C5-C4	2.43	118.28	113.62
31	B	607	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
31	b	611	CLA	C1D-ND-C4D	-2.43	104.61	106.33
31	n	602	CLA	C1D-ND-C4D	-2.43	104.61	106.33
31	s	603	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	c	502	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
31	r	612	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
31	B	613	CLA	O2A-CGA-CBA	2.43	119.53	111.91
47	s	608	CHL	C2C-C3C-C4C	2.43	108.22	106.49
47	Y1	601	CHL	C1-C2-C3	-2.43	121.85	126.04
31	n1	610	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
44	D	405	PL9	C20-C19-C21	2.43	119.35	115.27
31	s	610	CLA	C2D-C1D-ND	2.43	111.89	110.10
31	n	610	CLA	C3D-C2D-C1D	-2.43	102.52	105.83
31	B1	608	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
50	Y1	623	NEX	C31-C30-C29	2.43	130.77	127.31
31	R1	602	CLA	O2A-CGA-CBA	2.43	119.52	111.91
40	b1	623	DGD	O5D-C1E-C2E	2.43	112.09	108.30
31	g	602	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	S	617	CLA	O2D-CGD-O1D	-2.43	119.10	123.84
31	b1	605	CLA	CMC-C2C-C3C	2.43	132.70	126.12
49	Y1	622	XAT	O4-C5-C18	-2.43	112.15	115.06
41	Y	624	LHG	O8-C23-C24	2.42	119.52	111.91
47	N	605	CHL	CMA-C3A-C4A	2.42	118.29	111.77
31	G	613	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	C	512	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	G1	613	CLA	CHA-C4D-ND	2.42	137.57	132.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	510	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
31	C	506	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	C1	505	CLA	C1-O2A-CGA	2.42	122.80	116.44
48	n	620	LUT	C22-C23-C24	-2.42	108.98	111.74
37	B1	620	C7Z	C28-C27-C26	-2.42	120.40	127.20
33	B1	619	BCR	C37-C22-C21	-2.42	119.53	122.92
31	r1	604	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	b1	606	CLA	C1-O2A-CGA	2.42	122.80	116.44
31	B	615	CLA	C2D-C1D-ND	2.42	111.89	110.10
48	r	620	LUT	C3-C4-C5	-2.42	107.03	111.85
33	C	514	BCR	C33-C5-C4	2.42	118.27	113.62
31	s	612	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
31	S	614	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	C1	511	CLA	CHA-C4D-ND	2.42	137.56	132.50
33	C1	517	BCR	C19-C18-C17	2.42	122.66	118.94
31	g	611	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
31	C1	509	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
31	s1	604	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	S1	610	CLA	O2A-CGA-CBA	2.42	119.50	111.91
31	S1	614	CLA	C2D-C1D-ND	2.42	111.89	110.10
31	Y1	602	CLA	CMB-C2B-C3B	2.42	129.21	124.68
31	c1	511	CLA	O2A-CGA-CBA	2.42	119.50	111.91
31	a1	405	CLA	OBD-CAD-C3D	-2.42	122.69	128.52
47	G	609	CHL	CHC-C1C-NC	2.42	127.88	124.20
31	y1	611	CLA	CHD-C1D-ND	-2.42	122.23	124.45
31	B	606	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	A1	410	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	N1	610	CLA	C2C-C1C-NC	2.42	112.24	109.97
50	n	623	NEX	C4-C3-C2	2.42	115.44	110.77
31	C	509	CLA	O2A-CGA-CBA	2.42	119.50	111.91
35	b	622	LMG	O8-C28-C29	2.42	119.50	111.91
31	c1	513	CLA	CHA-C1A-NA	-2.42	120.86	126.40
31	r1	610	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
31	c1	507	CLA	C1-C2-C3	-2.42	121.86	126.04
31	a1	407	CLA	C2A-C1A-CHA	2.42	128.09	123.86
31	r	609	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	r	613	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	C	502	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	g	613	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
31	s1	611	CLA	O2A-CGA-CBA	2.42	119.49	111.91
31	y1	603	CLA	C1D-ND-C4D	-2.42	104.62	106.33
31	S1	617	CLA	O2D-CGD-O1D	-2.42	119.11	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	608	CLA	CMD-C2D-C3D	-2.42	122.06	127.61
31	y1	610	CLA	CMD-C2D-C3D	-2.42	122.06	127.61
45	F1	101	HEM	C1B-NB-C4B	2.42	107.57	105.07
31	b	616	CLA	CHA-C4D-ND	2.42	137.55	132.50
48	S	620	LUT	C35-C15-C14	-2.42	118.52	123.47
31	s	614	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
41	g1	624	LHG	O8-C23-C24	2.42	119.49	111.91
47	S	601	CHL	CHB-C4A-NA	2.42	127.85	124.51
33	C	515	BCR	C3-C4-C5	-2.42	109.76	114.08
31	N	610	CLA	CHA-C4D-ND	2.42	137.55	132.50
31	s	617	CLA	CHA-C4D-ND	2.42	137.55	132.50
31	r	602	CLA	CHA-C4D-ND	2.42	137.55	132.50
44	d	405	PL9	C36-C34-C33	-2.42	116.23	121.12
31	d1	403	CLA	C2D-C1D-ND	2.42	111.88	110.10
49	g1	622	XAT	C6-C7-C8	-2.42	120.89	125.99
48	n	621	LUT	C15-C14-C13	-2.42	123.86	127.31
31	b	609	CLA	CMD-C2D-C3D	-2.42	122.06	127.61
31	B1	615	CLA	CHD-C1D-ND	-2.41	122.23	124.45
31	Y1	604	CLA	CHA-C4D-ND	2.41	137.55	132.50
50	S1	623	NEX	C26-C27-C28	-2.41	120.89	125.99
31	c	510	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
47	G1	601	CHL	C1-C2-C3	-2.41	121.87	126.04
31	Y	602	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
31	R	610	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
31	b	604	CLA	C2D-C1D-ND	2.41	111.88	110.10
41	d	410	LHG	C5-O7-C7	-2.41	111.85	117.79
31	A1	405	CLA	CHA-C1A-NA	-2.41	120.87	126.40
31	B	603	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
31	r	610	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
31	N	603	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
31	r	611	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
47	N	609	CHL	C1B-CHB-C4A	-2.41	125.34	130.12
47	g1	601	CHL	CHB-C4A-NA	2.41	127.85	124.51
31	n1	614	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	r1	608	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
31	r1	609	CLA	CHA-C4D-ND	2.41	137.54	132.50
41	s1	624	LHG	C5-O7-C7	-2.41	111.86	117.79
48	R	620	LUT	C2-C3-C4	-2.41	107.00	110.30
31	s1	612	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	b1	605	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
31	C1	513	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
31	G1	603	CLA	CMD-C2D-C3D	-2.41	122.07	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c1	503	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
31	g1	613	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	g	614	CLA	O2A-CGA-CBA	2.41	119.47	111.91
31	C	507	CLA	CMB-C2B-C3B	2.41	129.19	124.68
46	H1	101	RRX	C11-C12-C13	-2.41	119.65	126.42
47	g1	608	CHL	CHB-C4A-NA	2.41	127.84	124.51
31	y1	613	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
31	A	407	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
31	y	614	CLA	C2D-C1D-ND	2.41	111.88	110.10
31	g	610	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
31	A	406	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	c1	512	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	g1	610	CLA	CHA-C4D-ND	2.41	137.54	132.50
33	B	619	BCR	C30-C25-C26	-2.41	119.22	122.61
31	C	509	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	N	603	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	Y1	612	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	a1	407	CLA	CHA-C1A-NA	-2.41	120.88	126.40
47	G	605	CHL	CHB-C4A-NA	2.41	127.84	124.51
47	s1	601	CHL	C2C-C3C-C4C	2.41	108.20	106.49
57	y1	627	PTY	C6-O7-C8	-2.41	113.41	117.90
31	R	602	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	b	611	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	S1	613	CLA	CHA-C4D-ND	2.41	137.53	132.50
47	S	608	CHL	C1B-CHB-C4A	-2.41	125.35	130.12
31	y	610	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	Y	603	CLA	OBD-CAD-C3D	-2.41	122.73	128.52
31	r1	602	CLA	C1D-ND-C4D	-2.41	104.63	106.33
31	s1	603	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
47	Y	609	CHL	C1-C2-C3	-2.41	121.88	126.04
47	y	601	CHL	C3C-C4C-NC	-2.40	107.87	110.57
31	b	610	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
31	C1	513	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
31	d1	403	CLA	CHA-C1A-NA	-2.40	120.89	126.40
31	c	509	CLA	C2D-C1D-ND	2.40	111.88	110.10
31	r1	602	CLA	CHA-C4D-ND	2.40	137.53	132.50
48	G1	620	LUT	C38-C25-C24	-2.40	118.41	123.56
31	B1	613	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	c1	503	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	b1	608	CLA	O2A-CGA-CBA	2.40	119.45	111.91
31	B1	615	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
31	y	611	CLA	C2D-C1D-ND	2.40	111.88	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	611	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	c1	501	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	B1	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
31	g1	611	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
47	g1	609	CHL	C4D-CHA-C1A	2.40	124.17	121.25
31	g	610	CLA	C2C-C1C-NC	2.40	112.22	109.97
31	R	602	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
33	B	619	BCR	C35-C13-C12	2.40	121.86	118.08
31	C	505	CLA	CHD-C1D-ND	-2.40	122.25	124.45
47	N	609	CHL	CHD-C4C-C3C	2.40	128.37	124.84
31	Y	611	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
31	a	405	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
31	R	609	CLA	CHA-C1A-NA	-2.40	120.90	126.40
31	c1	511	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
49	y	622	XAT	C20-C13-C14	-2.40	119.56	122.92
31	n	604	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	N1	604	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	G1	613	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	s	604	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	g1	603	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	s1	602	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	c1	503	CLA	O2A-CGA-CBA	2.40	119.43	111.91
31	y1	610	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	b	606	CLA	C2D-C1D-ND	2.40	111.87	110.10
31	N1	613	CLA	O2A-CGA-CBA	2.40	119.43	111.91
31	S	604	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
47	y1	605	CHL	CHB-C4A-NA	2.40	127.83	124.51
31	s	610	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	S1	617	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	g1	602	CLA	O2A-CGA-CBA	2.40	119.43	111.91
31	Y1	602	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	g1	604	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	S	614	CLA	O2A-CGA-CBA	2.40	119.43	111.91
31	c	507	CLA	C2D-C1D-ND	2.40	111.87	110.10
31	s	611	CLA	CHA-C1A-NA	-2.40	120.91	126.40
31	b	612	CLA	CAA-C2A-C3A	-2.40	106.22	112.78
31	B1	616	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
31	s	617	CLA	C1D-ND-C4D	-2.40	104.63	106.33
31	s1	612	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
35	C1	521	LMG	C8-O7-C10	-2.40	111.89	117.79
41	g1	624	LHG	C6-C5-C4	-2.40	106.12	111.79
31	g	610	CLA	CHA-C4D-ND	2.39	137.51	132.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	609	CLA	CHA-C4D-ND	2.39	137.51	132.50
31	S1	617	CLA	O2A-CGA-CBA	2.39	119.42	111.91
31	S1	602	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
31	N1	611	CLA	O2A-CGA-CBA	2.39	119.42	111.91
31	R	610	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
31	g	603	CLA	CHA-C4D-ND	2.39	137.51	132.50
31	c1	504	CLA	CHA-C4D-ND	2.39	137.51	132.50
38	b1	625	DGA	OG1-CA1-CA2	2.39	119.42	111.91
31	C	508	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	Y1	604	CLA	C1D-ND-C4D	-2.39	104.64	106.33
31	n	604	CLA	CMB-C2B-C1B	-2.39	124.79	128.46
49	n1	622	XAT	C20-C13-C14	-2.39	119.57	122.92
31	c	509	CLA	CHA-C1A-NA	-2.39	120.92	126.40
48	n	620	LUT	C18-C5-C6	-2.39	121.84	124.53
40	B1	623	DGD	C3G-C2G-C1G	-2.39	106.13	111.79
31	N1	613	CLA	C1-C2-C3	-2.39	121.91	126.04
47	G1	605	CHL	C1-O2A-CGA	2.39	123.68	116.73
34	a	412	SQD	O3-C3-C2	-2.39	104.82	110.35
31	S	602	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	N	602	CLA	C1D-ND-C4D	-2.39	104.64	106.33
33	B	619	BCR	C1-C6-C5	-2.39	119.25	122.61
49	n1	622	XAT	C18-C5-C6	-2.39	118.25	122.26
31	c	507	CLA	CHA-C1A-NA	-2.39	120.92	126.40
47	g1	608	CHL	C4A-NA-C1A	2.39	107.78	106.71
47	Y1	609	CHL	CHB-C4A-NA	2.39	127.82	124.51
31	y	603	CLA	C1D-ND-C4D	-2.39	104.64	106.33
31	N	614	CLA	CHA-C4D-ND	2.39	137.50	132.50
47	N1	605	CHL	CHD-C4C-C3C	2.39	128.35	124.84
31	G	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	n1	602	CLA	CHA-C4D-ND	2.39	137.50	132.50
41	N	624	LHG	O8-C23-C24	2.39	119.41	111.91
31	c1	507	CLA	C2D-C1D-ND	2.39	111.86	110.10
31	B1	613	CLA	CHD-C1D-ND	-2.39	122.26	124.45
31	r1	609	CLA	O2A-CGA-CBA	2.39	119.41	111.91
33	d1	404	BCR	C37-C22-C21	-2.39	119.58	122.92
31	c	511	CLA	CHA-C4D-ND	2.39	137.50	132.50
48	S	621	LUT	C38-C25-C24	-2.39	118.45	123.56
31	n	602	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
31	G	602	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
31	S1	610	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
50	G	623	NEX	C38-C25-C26	-2.39	118.26	122.26
31	g	613	CLA	C1-O2A-CGA	2.39	122.71	116.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	G	621	LUT	C35-C34-C33	-2.39	123.90	127.31
31	C	507	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
32	a	409	PHO	CMC-C2C-C3C	2.39	129.44	124.94
31	b	606	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
31	r	610	CLA	C1D-ND-C4D	-2.39	104.64	106.33
31	n	602	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
47	Y1	605	CHL	CHB-C4A-NA	2.39	127.81	124.51
31	y1	611	CLA	C2D-C1D-ND	2.39	111.86	110.10
49	y1	622	XAT	C38-C25-C26	-2.39	118.26	122.26
31	b	610	CLA	O2A-CGA-CBA	2.39	119.39	111.91
48	Y	621	LUT	C31-C30-C29	-2.39	123.91	127.31
31	n1	611	CLA	CHA-C4D-ND	2.38	137.49	132.50
31	b1	616	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
31	c	505	CLA	O2A-CGA-CBA	2.38	119.39	111.91
31	B1	608	CLA	O2A-CGA-CBA	2.38	119.39	111.91
31	n1	610	CLA	CHA-C4D-ND	2.38	137.49	132.50
31	n1	614	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
45	f1	101	HEM	C1B-NB-C4B	2.38	107.53	105.07
48	Y1	621	LUT	C35-C15-C14	-2.38	118.59	123.47
31	B1	602	CLA	C1-C2-C3	-2.38	121.92	126.04
35	b1	622	LMG	O8-C28-C29	2.38	119.39	111.91
41	G1	624	LHG	O8-C23-C24	2.38	119.38	111.91
31	D1	403	CLA	C6-C5-C3	-2.38	107.21	113.45
48	n1	621	LUT	C19-C9-C10	-2.38	119.59	122.92
49	N1	622	XAT	C39-C29-C30	-2.38	119.59	122.92
31	b1	615	CLA	CMA-C3A-C4A	2.38	118.17	111.77
31	b1	606	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
31	R	610	CLA	C1D-ND-C4D	-2.38	104.64	106.33
33	C1	514	BCR	C34-C9-C10	-2.38	119.59	122.92
31	r	603	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
47	Y1	605	CHL	C4D-CHA-C1A	2.38	124.15	121.25
31	b1	611	CLA	CHA-C4D-ND	2.38	137.48	132.50
31	b	612	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
48	G1	621	LUT	C38-C25-C24	-2.38	118.47	123.56
31	C1	504	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
31	c	511	CLA	C1D-ND-C4D	-2.38	104.64	106.33
32	A1	409	PHO	CMC-C2C-C3C	2.38	129.43	124.94
31	y1	612	CLA	CMA-C3A-C4A	2.38	118.17	111.77
31	B1	603	CLA	CHA-C4D-ND	2.38	137.48	132.50
31	y1	604	CLA	CHA-C4D-ND	2.38	137.48	132.50
31	b	605	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
31	s1	611	CLA	C1-C2-C3	-2.38	121.93	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	403	CLA	CHA-C4D-ND	2.38	137.48	132.50
31	G	603	CLA	C1D-ND-C4D	-2.38	104.64	106.33
52	S	626	3PH	O31-C31-C32	2.38	119.37	111.91
31	S1	610	CLA	OBD-CAD-C3D	-2.38	122.80	128.52
31	Y	608	CLA	O2A-CGA-CBA	2.38	119.37	111.91
31	G	613	CLA	O2A-CGA-CBA	2.38	119.37	111.91
31	n1	604	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
31	c	508	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	g	610	CLA	C1D-ND-C4D	-2.38	104.65	106.33
31	b1	611	CLA	C1D-ND-C4D	-2.38	104.65	106.33
31	s	610	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
31	N1	614	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
31	s1	612	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
44	d1	405	PL9	C27-C28-C29	-2.38	121.94	127.66
31	r1	604	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
31	G	611	CLA	C1D-ND-C4D	-2.38	104.65	106.33
47	Y	606	CHL	C1-O2A-CGA	2.38	122.68	116.44
47	N1	607	CHL	C1-O2A-CGA	2.38	122.68	116.44
46	H	101	RRX	C15-C16-C17	-2.38	118.61	123.47
48	y1	621	LUT	C18-C5-C6	-2.38	121.86	124.53
31	n	602	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	b1	604	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	b	616	CLA	CHA-C1A-NA	-2.38	120.96	126.40
31	G1	602	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
47	N1	609	CHL	CHD-C4C-C3C	2.38	128.33	124.84
31	s1	605	CLA	C2D-C1D-ND	2.37	111.85	110.10
31	g1	610	CLA	O2A-CGA-CBA	2.37	119.36	111.91
31	B	606	CLA	CMB-C2B-C3B	2.37	129.12	124.68
31	n	602	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
31	S1	602	CLA	CHA-C4D-ND	2.37	137.47	132.50
33	c1	514	BCR	C23-C24-C25	-2.37	120.53	127.20
31	Y	613	CLA	CMB-C2B-C3B	2.37	129.12	124.68
31	c	513	CLA	CHA-C4D-ND	2.37	137.46	132.50
50	s	623	NEX	C38-C25-C26	-2.37	118.28	122.26
31	a	410	CLA	C2D-C1D-ND	2.37	111.85	110.10
31	S1	609	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
33	B1	619	BCR	C36-C18-C17	-2.37	119.60	122.92
49	N	622	XAT	C6-C7-C8	-2.37	120.98	125.99
45	F	101	HEM	CBA-CAA-C2A	-2.37	108.57	112.62
31	B	609	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
31	y	604	CLA	C1-O2A-CGA	2.37	122.67	116.44
31	A1	410	CLA	O2D-CGD-O1D	-2.37	119.20	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g1	603	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
37	b1	620	C7Z	C8-C7-C6	-2.37	120.54	127.20
31	B	602	CLA	CHA-C1A-NA	-2.37	120.97	126.40
31	s	605	CLA	C1-O2A-CGA	2.37	122.67	116.44
31	c	507	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
31	c	511	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
50	r1	622	NEX	C39-C29-C30	-2.37	119.60	122.92
44	d	405	PL9	C20-C19-C21	2.37	119.26	115.27
31	C	503	CLA	C1D-ND-C4D	-2.37	104.65	106.33
31	C1	509	CLA	CMB-C2B-C3B	2.37	129.11	124.68
47	N	609	CHL	C1-C2-C3	-2.37	121.94	126.04
31	n1	614	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
31	R	602	CLA	O2A-CGA-CBA	2.37	119.34	111.91
31	n	614	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	r1	610	CLA	C1D-ND-C4D	-2.37	104.65	106.33
31	N	610	CLA	CHD-C1D-ND	-2.37	122.28	124.45
31	N	613	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
31	a1	405	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
31	b1	609	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
31	Y1	614	CLA	CMB-C2B-C3B	2.37	129.11	124.68
31	b	614	CLA	C1D-ND-C4D	-2.37	104.65	106.33
47	s1	608	CHL	CHD-C4C-C3C	2.37	128.32	124.84
47	y1	606	CHL	C1-C2-C3	-2.37	121.95	126.04
31	S	603	CLA	CHA-C1A-NA	-2.37	120.98	126.40
47	G1	601	CHL	C1B-CHB-C4A	-2.37	125.43	130.12
47	Y	601	CHL	C4A-NA-C1A	2.37	107.77	106.71
31	b1	606	CLA	C2D-C1D-ND	2.37	111.85	110.10
31	N1	610	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
31	C1	503	CLA	O2A-CGA-CBA	2.37	119.33	111.91
31	b1	603	CLA	CHA-C4D-ND	2.37	137.45	132.50
47	Y1	609	CHL	C1-C2-C3	-2.37	121.95	126.04
31	B1	609	CLA	CHD-C1D-ND	-2.37	122.28	124.45
31	Y	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
47	r1	606	CHL	CHB-C4A-NA	2.37	127.78	124.51
31	c	506	CLA	CHA-C4D-ND	2.37	137.45	132.50
31	S1	602	CLA	O1D-CGD-CBD	-2.36	119.64	124.48
31	c1	510	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
31	B	617	CLA	CHA-C4D-ND	2.36	137.44	132.50
34	A	412	SQD	O3-C3-C2	-2.36	104.88	110.35
31	B	605	CLA	C1-O2A-CGA	2.36	122.65	116.44
31	r	611	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
46	H	101	RRX	C11-C12-C13	-2.36	119.78	126.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	g1	606	CHL	C1-O2A-CGA	2.36	122.64	116.44
48	Y	621	LUT	C31-C32-C33	-2.36	119.78	126.42
47	N	608	CHL	CHB-C4A-NA	2.36	127.78	124.51
31	C1	507	CLA	CAC-C3C-C4C	2.36	127.88	124.81
31	b	607	CLA	CMA-C3A-C4A	2.36	118.12	111.77
31	S	609	CLA	CMC-C2C-C1C	2.36	128.64	125.04
31	C	507	CLA	C1-C2-C3	-2.36	121.96	126.04
31	Y	611	CLA	CHA-C1A-NA	-2.36	120.99	126.40
31	R	604	CLA	CMB-C2B-C3B	2.36	129.10	124.68
47	R	607	CHL	C1-O2A-CGA	2.36	122.64	116.44
47	N1	601	CHL	CHD-C4C-C3C	2.36	128.31	124.84
49	Y	622	XAT	C18-C5-C6	-2.36	118.30	122.26
47	N	605	CHL	CHB-C4A-NA	2.36	127.78	124.51
31	C	505	CLA	OBD-CAD-C3D	-2.36	122.84	128.52
47	g1	609	CHL	C3C-C4C-NC	-2.36	107.92	110.57
31	N	602	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	s	609	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	c1	510	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	D	403	CLA	C1D-ND-C4D	-2.36	104.66	106.33
35	H	102	LMG	O8-C28-C29	2.36	119.31	111.91
31	b	603	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
47	s1	608	CHL	CHB-C4A-NA	2.36	127.77	124.51
44	D	405	PL9	C7-C8-C9	-2.36	122.86	126.79
31	C1	502	CLA	CHA-C4D-ND	2.36	137.43	132.50
31	A1	407	CLA	CHA-C4D-ND	2.36	137.43	132.50
33	A	411	BCR	C34-C9-C10	-2.36	119.62	122.92
47	y	609	CHL	C4A-NA-C1A	2.36	107.77	106.71
31	S1	614	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
49	r1	621	XAT	C6-C7-C8	-2.36	121.01	125.99
48	y	620	LUT	C15-C14-C13	-2.36	123.95	127.31
31	C	509	CLA	CMB-C2B-C3B	2.36	129.09	124.68
31	Y	614	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
55	r1	625	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
31	R1	608	CLA	C1-C2-C3	-2.36	121.97	126.04
41	Y	624	LHG	C6-C5-C4	-2.36	106.21	111.79
31	g	610	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
31	S1	612	CLA	C1D-ND-C4D	-2.36	104.66	106.33
31	B1	611	CLA	CHA-C4D-ND	2.36	137.43	132.50
31	b1	611	CLA	O2A-CGA-CBA	2.36	119.30	111.91
31	B	608	CLA	O2A-CGA-CBA	2.36	119.30	111.91
31	Y1	608	CLA	C2D-C1D-ND	2.36	111.84	110.10
31	G	614	CLA	CMD-C2D-C3D	-2.36	122.20	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	610	CLA	C2C-C1C-NC	2.35	112.18	109.97
31	c	504	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
33	c1	514	BCR	C34-C9-C10	-2.35	119.62	122.92
31	B	612	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	G	614	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	S1	602	CLA	C1D-ND-C4D	-2.35	104.66	106.33
31	A1	406	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	B1	615	CLA	C2D-C1D-ND	2.35	111.84	110.10
31	G	603	CLA	CHA-C4D-ND	2.35	137.42	132.50
46	h1	101	RRX	C28-C27-C26	2.35	116.54	111.85
41	c	625	LHG	C5-O7-C7	-2.35	112.00	117.79
31	G1	604	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
47	S	606	CHL	CHB-C4A-NA	2.35	127.76	124.51
31	n1	612	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	B1	606	CLA	O2A-CGA-CBA	2.35	119.29	111.91
31	b	607	CLA	CAC-C3C-C4C	2.35	127.86	124.81
31	G	614	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
33	D1	404	BCR	C33-C5-C6	-2.35	121.89	124.53
31	B	614	CLA	CMB-C2B-C3B	2.35	129.08	124.68
44	D1	405	PL9	C8-C7-C3	2.35	118.62	111.98
31	B	607	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
35	c	521	LMG	O7-C10-O9	-2.35	118.02	123.70
31	B	602	CLA	O2A-CGA-CBA	2.35	119.28	111.91
31	y1	603	CLA	CHA-C4D-ND	2.35	137.41	132.50
31	R1	610	CLA	C2C-C1C-NC	2.35	112.17	109.97
48	S1	621	LUT	C31-C30-C29	-2.35	123.96	127.31
47	Y	605	CHL	C4D-CHA-C1A	2.35	124.11	121.25
31	r	604	CLA	CMA-C3A-C4A	2.35	118.09	111.77
48	G	621	LUT	C20-C13-C12	2.35	121.78	118.08
47	s1	607	CHL	C4A-NA-C1A	2.35	107.76	106.71
47	g	606	CHL	CHB-C4A-NA	2.35	127.76	124.51
37	b1	620	C7Z	C15-C35-C34	-2.35	118.66	123.47
33	C	514	BCR	C36-C18-C17	-2.35	119.63	122.92
31	s1	605	CLA	CHA-C1A-NA	-2.35	121.02	126.40
31	g1	611	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
31	N	603	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
31	c1	509	CLA	CHA-C4D-ND	2.35	137.41	132.50
47	s1	606	CHL	C4D-CHA-C1A	2.35	124.11	121.25
31	g	604	CLA	O2A-CGA-CBA	2.35	119.27	111.91
31	R1	603	CLA	O2A-CGA-CBA	2.35	119.27	111.91
31	B1	615	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
31	N	613	CLA	C1C-C2C-C3C	-2.35	104.49	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r1	609	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
37	B1	620	C7Z	C21-C26-C27	2.35	122.41	115.78
31	R	604	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
31	b	602	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
31	b1	610	CLA	C2D-C1D-ND	2.34	111.83	110.10
31	n	603	CLA	CMD-C2D-C3D	-2.34	122.22	127.61
31	a1	406	CLA	CMB-C2B-C3B	2.34	129.06	124.68
31	r1	610	CLA	CMA-C3A-C4A	2.34	118.08	111.77
31	b	604	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
31	R	608	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
31	S	609	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
31	C	511	CLA	C1-C2-C3	-2.34	121.99	126.04
33	a1	411	BCR	C38-C26-C25	-2.34	121.90	124.53
31	Y	611	CLA	CHA-C4D-ND	2.34	137.40	132.50
31	r	604	CLA	C1D-ND-C4D	-2.34	104.67	106.33
31	g1	602	CLA	C1D-ND-C4D	-2.34	104.67	106.33
33	D	404	BCR	C33-C5-C4	2.34	118.12	113.62
31	n	604	CLA	O2A-CGA-CBA	2.34	119.26	111.91
31	N1	611	CLA	CHA-C1A-NA	-2.34	121.03	126.40
50	G1	623	NEX	C11-C10-C9	2.34	130.65	127.31
47	y	606	CHL	CHD-C4C-C3C	2.34	128.28	124.84
47	n	605	CHL	CHB-C4A-NA	2.34	127.75	124.51
31	S	604	CLA	CHA-C4D-ND	2.34	137.40	132.50
47	G	608	CHL	C4D-CHA-C1A	2.34	124.10	121.25
35	a1	413	LMG	O8-C28-C29	2.34	119.26	111.91
47	r	606	CHL	C4A-NA-C1A	2.34	107.76	106.71
31	A	407	CLA	C2D-C1D-ND	2.34	111.83	110.10
31	Y1	614	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
31	r1	610	CLA	CHA-C4D-ND	2.34	137.40	132.50
47	N1	605	CHL	C1-O2A-CGA	2.34	122.59	116.44
31	s	605	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
56	R1	626	ERG	C4-C5-C10	2.34	119.53	116.42
48	n1	620	LUT	C35-C15-C14	-2.34	118.68	123.47
31	S	610	CLA	C2D-C1D-ND	2.34	111.83	110.10
49	g1	622	XAT	C18-C5-C6	-2.34	118.34	122.26
31	R1	603	CLA	CHA-C1A-NA	-2.34	121.04	126.40
31	y	611	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
33	A	411	BCR	C33-C5-C4	2.34	118.11	113.62
31	b	603	CLA	CHA-C4D-ND	2.34	137.39	132.50
31	a	407	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
31	n	602	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
48	S	621	LUT	C8-C7-C6	-2.34	120.64	127.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	606	CLA	C1D-ND-C4D	-2.34	104.67	106.33
31	B1	606	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
33	c1	517	BCR	C1-C6-C5	-2.34	119.32	122.61
31	a	410	CLA	O2A-CGA-CBA	2.34	119.24	111.91
41	g	624	LHG	O8-C23-C24	2.34	119.24	111.91
31	G1	611	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
31	n	613	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
31	c1	509	CLA	C1-C2-C3	-2.34	122.00	126.04
56	r1	626	ERG	C2-C3-C4	2.34	113.51	110.31
31	Y1	611	CLA	CMD-C2D-C3D	-2.34	122.24	127.61
31	r	609	CLA	CMA-C3A-C4A	2.34	118.05	111.77
31	d1	402	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
33	B1	618	BCR	C30-C25-C26	-2.34	119.32	122.61
48	s	620	LUT	C35-C15-C14	-2.34	118.69	123.47
31	s	602	CLA	CMA-C3A-C4A	2.34	118.05	111.77
38	B	625	DGA	OG1-CA1-CA2	2.34	119.24	111.91
47	r	607	CHL	C4A-NA-C1A	2.34	107.76	106.71
31	a1	405	CLA	C1D-ND-C4D	-2.34	104.68	106.33
47	n1	605	CHL	C1-C2-C3	-2.34	122.00	126.04
31	s	613	CLA	C1-O2A-CGA	2.34	122.57	116.44
31	N1	604	CLA	CHA-C1A-NA	-2.34	121.05	126.40
33	A	411	BCR	C36-C18-C17	-2.34	119.65	122.92
46	h1	101	RRX	C16-C15-C14	2.33	128.26	123.47
31	C	508	CLA	C2D-C1D-ND	2.33	111.82	110.10
31	Y	602	CLA	C1D-ND-C4D	-2.33	104.68	106.33
31	N	610	CLA	C2C-C1C-NC	2.33	112.16	109.97
31	b	611	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
47	S1	601	CHL	C4A-NA-C1A	2.33	107.75	106.71
49	N	622	XAT	C18-C5-C6	-2.33	118.35	122.26
31	C1	506	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
31	r	612	CLA	CMA-C3A-C4A	2.33	118.04	111.77
31	y	614	CLA	CAA-CBA-CGA	-2.33	106.44	113.25
31	d1	403	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
31	B	612	CLA	C1D-ND-C4D	-2.33	104.68	106.33
33	C	516	BCR	C33-C5-C4	2.33	118.09	113.62
31	R	610	CLA	CHA-C4D-ND	2.33	137.37	132.50
31	b	617	CLA	CHA-C4D-ND	2.33	137.37	132.50
47	Y	607	CHL	C4D-CHA-C1A	2.33	124.08	121.25
49	n	622	XAT	C39-C29-C30	-2.33	119.66	122.92
31	A1	407	CLA	CAA-CBA-CGA	-2.33	106.44	113.25
45	f	101	HEM	C3D-C4D-ND	-2.33	107.57	110.17
31	S1	605	CLA	CMD-C2D-C3D	-2.33	122.25	127.61

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S1	605	CLA	C2D-C1D-ND	2.33	111.82	110.10
31	b1	612	CLA	CHD-C1D-ND	-2.33	122.31	124.45
31	R	604	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	n1	602	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	b	603	CLA	O2A-CGA-CBA	2.33	119.22	111.91
31	Y	608	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
31	N1	614	CLA	CHA-C4D-ND	2.33	137.37	132.50
31	B1	612	CLA	O2A-CGA-CBA	2.33	119.22	111.91
31	c1	511	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
31	S	605	CLA	C1-O2A-CGA	2.33	122.55	116.44
31	r1	612	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
47	R1	607	CHL	C1B-CHB-C4A	-2.33	125.51	130.12
33	C	515	BCR	C38-C26-C25	-2.33	121.91	124.53
31	b1	615	CLA	CHA-C1A-NA	-2.33	121.07	126.40
34	c1	526	SQD	O3-C3-C2	-2.33	104.97	110.35
31	N1	602	CLA	C3D-C2D-C1D	-2.33	102.66	105.83
41	Y1	624	LHG	C6-C5-C4	-2.33	106.28	111.79
31	C	513	CLA	CHA-C4D-ND	2.33	137.37	132.50
31	c	504	CLA	CHA-C4D-ND	2.33	137.37	132.50
31	n1	613	CLA	CHA-C1A-NA	-2.33	121.07	126.40
31	R1	603	CLA	C2D-C1D-ND	2.33	111.82	110.10
33	C	517	BCR	C23-C24-C25	-2.33	120.67	127.20
31	S	613	CLA	O2A-CGA-CBA	2.33	119.21	111.91
31	g1	602	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
31	r	612	CLA	CHA-C1A-NA	-2.33	121.07	126.40
47	G	607	CHL	CMB-C2B-C1B	-2.33	124.89	128.46
49	y1	622	XAT	O24-C25-C38	-2.33	112.27	115.06
48	n1	620	LUT	C38-C25-C24	-2.32	118.58	123.56
31	c	505	CLA	C2D-C1D-ND	2.32	111.82	110.10
48	Y1	620	LUT	C20-C13-C14	-2.32	119.67	122.92
31	G	602	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
31	b1	607	CLA	CHA-C4D-ND	2.32	137.36	132.50
31	s	610	CLA	O2A-CGA-CBA	2.32	119.20	111.91
31	b	617	CLA	C1-O2A-CGA	2.32	122.54	116.44
31	G	604	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
50	N	623	NEX	C31-C30-C29	2.32	130.63	127.31
47	Y1	609	CHL	CHD-C4C-C3C	2.32	128.25	124.84
31	B	611	CLA	CHA-C4D-ND	2.32	137.36	132.50
34	A1	412	SQD	O3-C3-C2	-2.32	104.98	110.35
31	s	617	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	d1	402	CLA	C1D-ND-C4D	-2.32	104.69	106.33
31	s1	614	CLA	C1-C2-C3	-2.32	122.03	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	602	CLA	O2A-CGA-CBA	2.32	119.20	111.91
50	R	622	NEX	C20-C13-C14	-2.32	119.67	122.92
31	S1	603	CLA	CHA-C1A-NA	-2.32	121.08	126.40
31	Y	614	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	c1	502	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
31	n	602	CLA	CMC-C2C-C1C	2.32	128.57	125.04
31	R	604	CLA	C2D-C1D-ND	2.32	111.81	110.10
49	R	621	XAT	C20-C13-C14	-2.32	119.67	122.92
48	s	621	LUT	C38-C25-C24	-2.32	118.59	123.56
31	y1	613	CLA	O2A-CGA-CBA	2.32	119.19	111.91
48	R1	620	LUT	C8-C7-C6	-2.32	120.68	127.20
33	c1	517	BCR	C35-C13-C12	2.32	121.73	118.08
31	N1	602	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
31	R1	609	CLA	CHA-C4D-ND	2.32	137.35	132.50
48	n1	620	LUT	C10-C11-C12	-2.32	115.98	123.22
31	c1	511	CLA	C1D-ND-C4D	-2.32	104.69	106.33
31	r1	602	CLA	C6-C5-C3	-2.32	107.37	113.45
31	Y1	612	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	S1	611	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	c	502	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
31	b	604	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	Y1	613	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	N1	612	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
48	g1	620	LUT	C38-C25-C24	-2.32	118.60	123.56
31	G1	613	CLA	C1D-ND-C4D	-2.32	104.69	106.33
31	s	602	CLA	CAC-C3C-C4C	2.32	127.82	124.81
31	R	610	CLA	CAA-C2A-C3A	-2.32	106.43	112.78
31	N1	602	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
33	d1	404	BCR	C38-C26-C27	2.32	118.06	113.62
31	n1	611	CLA	CMA-C3A-C4A	2.32	118.00	111.77
31	b1	609	CLA	C2A-C1A-CHA	2.32	127.91	123.86
31	A1	407	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
31	y1	611	CLA	CMA-C3A-C4A	2.32	118.00	111.77
31	C1	511	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
31	a	405	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
31	C	503	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
31	g	602	CLA	CHA-C1A-NA	-2.31	121.10	126.40
31	Y	602	CLA	CMC-C2C-C1C	2.31	128.56	125.04
31	y1	613	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
48	N1	621	LUT	C35-C15-C14	-2.31	118.73	123.47
31	D1	402	CLA	CHA-C4D-ND	2.31	137.34	132.50
31	C1	513	CLA	C1C-C2C-C3C	-2.31	104.52	106.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	512	CLA	C1-C2-C3	-2.31	122.04	126.04
31	n1	602	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
31	c	506	CLA	CHA-C1A-NA	-2.31	121.10	126.40
31	c1	509	CLA	C1D-ND-C4D	-2.31	104.69	106.33
31	s1	612	CLA	C1D-ND-C4D	-2.31	104.69	106.33
47	g	609	CHL	CHD-C4C-C3C	2.31	128.24	124.84
31	B	617	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
31	r	608	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
33	b1	618	BCR	C30-C25-C26	-2.31	119.36	122.61
31	a	405	CLA	CHA-C4D-ND	2.31	137.34	132.50
31	R	609	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
47	s1	606	CHL	CMB-C2B-C1B	-2.31	124.91	128.46
31	a	405	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
31	s1	611	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
48	g1	621	LUT	C38-C25-C24	-2.31	118.61	123.56
31	a1	407	CLA	CMB-C2B-C3B	2.31	129.00	124.68
31	s1	617	CLA	CHA-C4D-ND	2.31	137.33	132.50
49	n1	622	XAT	C39-C29-C30	-2.31	119.69	122.92
31	S	605	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
31	Y	612	CLA	C1D-ND-C4D	-2.31	104.69	106.33
31	c	512	CLA	C1-O2A-CGA	2.31	122.50	116.44
31	A	405	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
31	C	503	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
31	c1	503	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
31	G1	602	CLA	CHA-C4D-ND	2.31	137.33	132.50
47	s	608	CHL	C1-C2-C3	-2.31	122.05	126.04
47	s	607	CHL	C1B-CHB-C4A	-2.31	125.54	130.12
31	A	406	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
47	N1	606	CHL	C1B-CHB-C4A	-2.31	125.55	130.12
49	G	622	XAT	O4-C5-C4	-2.31	111.65	113.38
49	r1	621	XAT	C32-C33-C34	2.31	122.48	118.94
31	D1	402	CLA	CHA-C1A-NA	-2.31	121.11	126.40
49	N	622	XAT	O4-C5-C18	-2.31	112.29	115.06
31	b1	610	CLA	C1-C2-C3	-2.31	122.05	126.04
31	c	508	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
31	B1	610	CLA	C1D-ND-C4D	-2.31	104.70	106.33
48	r	620	LUT	C2-C3-C4	-2.31	107.15	110.30
31	c1	511	CLA	CHA-C1A-NA	-2.31	121.11	126.40
31	B1	617	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
31	B1	609	CLA	CHA-C1A-NA	-2.31	121.12	126.40
31	C	510	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
31	Y1	613	CLA	C1-O2A-CGA	2.31	122.49	116.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	602	CLA	O1D-CGD-CBD	-2.31	119.77	124.48
31	S	612	CLA	CHD-C1D-ND	-2.31	122.33	124.45
31	N	613	CLA	CMB-C2B-C3B	2.31	128.99	124.68
37	b	620	C7Z	C7-C8-C9	-2.31	122.75	126.23
31	s	617	CLA	CHA-C1A-NA	-2.31	121.12	126.40
40	C	519	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
31	S	603	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
37	B	620	C7Z	C19-C9-C10	-2.31	119.69	122.92
31	B1	607	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
31	S	613	CLA	C1-O2A-CGA	2.30	122.49	116.44
31	Y1	610	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
47	n1	609	CHL	CMB-C2B-C1B	-2.30	124.92	128.46
31	s1	612	CLA	CMA-C3A-C4A	2.30	117.97	111.77
32	a	408	PHO	C1-C2-C3	-2.30	122.06	126.04
34	b1	626	SQD	O3-C3-C2	-2.30	105.02	110.35
31	R	603	CLA	CAC-C3C-C4C	2.30	127.80	124.81
31	b1	602	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
31	A1	410	CLA	O2A-CGA-CBA	2.30	119.14	111.91
47	N1	608	CHL	CMB-C2B-C1B	-2.30	124.92	128.46
31	C	512	CLA	O2A-CGA-CBA	2.30	119.14	111.91
31	c1	501	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
33	B1	619	BCR	C8-C7-C6	-2.30	120.73	127.20
31	c1	507	CLA	CHA-C1A-NA	-2.30	121.12	126.40
31	N	604	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
31	B	608	CLA	C1-C2-C3	-2.30	122.06	126.04
31	S1	614	CLA	CMA-C3A-C4A	2.30	117.96	111.77
47	Y1	609	CHL	C1-O2A-CGA	2.30	122.48	116.44
31	C	512	CLA	CHA-C1A-NA	-2.30	121.13	126.40
47	Y1	601	CHL	CMB-C2B-C1B	-2.30	124.93	128.46
31	G1	614	CLA	O2A-CGA-CBA	2.30	119.13	111.91
31	a1	406	CLA	CHA-C4D-ND	2.30	137.31	132.50
31	A1	406	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
31	Y1	608	CLA	CHA-C1A-NA	-2.30	121.13	126.40
31	r	608	CLA	C2D-C1D-ND	2.30	111.80	110.10
31	g	604	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
47	Y	607	CHL	CMB-C2B-C1B	-2.30	124.93	128.46
56	R1	626	ERG	C20-C22-C23	-2.30	118.53	125.67
31	S1	610	CLA	CMC-C2C-C1C	2.30	128.54	125.04
47	S1	608	CHL	C2C-C3C-C4C	2.30	108.13	106.49
34	M1	101	SQD	O3-C3-C2	-2.30	105.03	110.35
31	B1	608	CLA	C2D-C1D-ND	2.30	111.80	110.10
31	B1	609	CLA	O1D-CGD-CBD	-2.30	119.78	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Y1	607	CHL	C4D-CHA-C1A	2.30	124.05	121.25
47	n	607	CHL	CMB-C2B-C1B	-2.30	124.93	128.46
37	B1	620	C7Z	C11-C12-C13	-2.30	119.96	126.42
31	b1	605	CLA	C1-C2-C3	-2.30	122.07	126.04
31	r	613	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
31	N1	604	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
31	b1	602	CLA	CHA-C1A-NA	-2.30	121.13	126.40
50	R1	622	NEX	C31-C30-C29	2.30	130.59	127.31
47	y	605	CHL	CHB-C4A-NA	2.30	127.69	124.51
31	G1	604	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
31	c1	505	CLA	CHA-C1A-NA	-2.30	121.14	126.40
47	r	607	CHL	C1-O2A-CGA	2.30	122.47	116.44
47	G1	607	CHL	CMB-C2B-C1B	-2.30	124.93	128.46
31	s	612	CLA	C1D-ND-C4D	-2.30	104.70	106.33
31	C1	503	CLA	CMB-C2B-C3B	2.30	128.98	124.68
49	N1	622	XAT	C28-C29-C30	2.30	122.47	118.94
31	a1	405	CLA	CMA-C3A-C4A	2.30	117.95	111.77
31	s	612	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
31	a	405	CLA	C6-C5-C3	-2.30	107.43	113.45
31	R	610	CLA	CHA-C1A-NA	-2.30	121.14	126.40
31	y1	611	CLA	CHA-C1A-NA	-2.30	121.14	126.40
31	C	501	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
31	S1	612	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
50	n1	623	NEX	C31-C32-C33	2.30	132.87	126.42
31	N	603	CLA	OBD-CAD-C3D	-2.30	122.99	128.52
31	a1	407	CLA	O2A-CGA-CBA	2.30	119.11	111.91
50	N	623	NEX	C19-C9-C10	-2.30	119.71	122.92
31	s	602	CLA	CHA-C4D-ND	2.30	137.30	132.50
31	G1	602	CLA	CHD-C1D-ND	-2.29	122.34	124.45
31	G	613	CLA	CMD-C2D-C3D	-2.29	122.33	127.61
31	G1	610	CLA	CAA-C2A-C3A	-2.29	106.49	112.78
31	n1	611	CLA	C1D-ND-C4D	-2.29	104.70	106.33
48	y	620	LUT	C19-C9-C10	-2.29	119.71	122.92
31	a1	407	CLA	CHA-C4D-ND	2.29	137.30	132.50
31	c1	511	CLA	C2A-C1A-CHA	2.29	127.87	123.86
50	G1	623	NEX	C19-C9-C10	-2.29	119.71	122.92
47	r	606	CHL	C3C-C4C-NC	-2.29	108.00	110.57
33	b	618	BCR	C15-C14-C13	-2.29	124.04	127.31
48	n1	621	LUT	C38-C25-C24	-2.29	118.65	123.56
47	R1	607	CHL	C4A-NA-C1A	2.29	107.74	106.71
47	n	605	CHL	C4D-CHA-C1A	2.29	124.04	121.25
31	c1	506	CLA	O2A-CGA-CBA	2.29	119.10	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	D	405	PL9	C36-C34-C33	-2.29	116.48	121.12
47	y1	601	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
33	C1	516	BCR	C19-C18-C17	2.29	122.46	118.94
31	B1	613	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
33	b	619	BCR	C27-C26-C25	-2.29	119.40	122.73
47	g	607	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
31	N1	613	CLA	C1-O2A-CGA	2.29	122.46	116.44
31	n1	614	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
31	C	503	CLA	CHA-C1A-NA	-2.29	121.15	126.40
47	g1	601	CHL	C4D-CHA-C1A	2.29	124.04	121.25
31	g1	602	CLA	C2C-C1C-NC	2.29	112.12	109.97
31	g1	610	CLA	C1D-ND-C4D	-2.29	104.71	106.33
31	S	611	CLA	C1-C2-C3	-2.29	122.08	126.04
47	n	609	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
47	g1	609	CHL	CHB-C4A-NA	2.29	127.68	124.51
31	y1	604	CLA	O2A-CGA-CBA	2.29	119.09	111.91
31	R	612	CLA	C1D-ND-C4D	-2.29	104.71	106.33
31	g1	603	CLA	C1D-ND-C4D	-2.29	104.71	106.33
47	y	607	CHL	CMB-C2B-C1B	-2.29	124.95	128.46
31	g	610	CLA	CMB-C2B-C3B	2.29	128.96	124.68
34	m1	101	SQD	O3-C3-C2	-2.29	105.06	110.35
47	s1	608	CHL	C4D-CHA-C1A	2.29	124.03	121.25
31	N	614	CLA	O2A-CGA-CBA	2.29	119.09	111.91
31	r	603	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	s	609	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	r1	603	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	g1	612	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
50	y	623	NEX	C31-C32-C33	2.29	132.84	126.42
37	B1	620	C7Z	C38-C25-C24	2.29	118.59	114.36
31	n1	614	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
48	Y	621	LUT	C2-C3-C4	-2.29	107.17	110.30
31	A	407	CLA	C1-O2A-CGA	2.29	122.44	116.44
32	a1	409	PHO	CMC-C2C-C3C	2.29	129.25	124.94
31	r1	602	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
47	R	606	CHL	C4A-NA-C1A	2.29	107.73	106.71
47	G1	609	CHL	CHC-C1C-NC	2.29	127.67	124.20
34	C	526	SQD	O3-C3-C2	-2.29	105.06	110.35
31	n	611	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	C	505	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
31	R1	604	CLA	C1-O2A-CGA	2.29	122.44	116.44
35	d	411	LMG	O1-C1-C2	2.29	111.87	108.30
33	b1	619	BCR	C34-C9-C10	-2.29	119.72	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	s1	621	LUT	C19-C9-C10	-2.29	119.72	122.92
50	n1	623	NEX	C19-C9-C10	-2.29	119.72	122.92
33	b	618	BCR	C4-C5-C6	-2.29	119.41	122.73
33	c	517	BCR	C2-C1-C6	2.29	114.00	110.48
31	b1	610	CLA	O2A-CGA-CBA	2.29	119.08	111.91
47	y1	606	CHL	C4D-CHA-C1A	2.28	124.03	121.25
47	n1	607	CHL	CMB-C2B-C1B	-2.28	124.95	128.46
46	h1	101	RRX	C15-C14-C13	-2.28	124.05	127.31
31	g	604	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
31	B	613	CLA	C2D-C1D-ND	2.28	111.79	110.10
49	G1	622	XAT	C40-C33-C34	-2.28	119.72	122.92
47	Y1	607	CHL	CMB-C2B-C1B	-2.28	124.95	128.46
31	C	502	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
31	A	410	CLA	OBD-CAD-C3D	-2.28	123.03	128.52
33	C1	516	BCR	C23-C24-C25	-2.28	120.79	127.20
31	b1	612	CLA	CHA-C4D-ND	2.28	137.27	132.50
31	N1	604	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
31	B	610	CLA	CHA-C1A-NA	-2.28	121.17	126.40
31	s	605	CLA	CHA-C1A-NA	-2.28	121.17	126.40
31	b1	612	CLA	CMB-C2B-C3B	2.28	128.95	124.68
47	G	605	CHL	C4A-NA-C1A	2.28	107.73	106.71
31	c	506	CLA	O2A-CGA-CBA	2.28	119.07	111.91
48	r	620	LUT	C18-C5-C6	-2.28	121.97	124.53
31	C1	512	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
31	b	613	CLA	O2A-CGA-CBA	2.28	119.06	111.91
47	g1	607	CHL	CMB-C2B-C1B	-2.28	124.96	128.46
31	b1	604	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
31	b1	617	CLA	CHA-C1A-NA	-2.28	121.18	126.40
47	r1	607	CHL	C1-O2A-CGA	2.28	122.42	116.44
56	R1	626	ERG	C11-C9-C10	2.28	119.23	113.58
31	y	602	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
47	n	609	CHL	C2C-C3C-C4C	2.28	108.11	106.49
31	D	402	CLA	C2C-C1C-NC	2.28	112.11	109.97
31	B1	617	CLA	CMA-C3A-C4A	2.28	117.89	111.77
31	C	506	CLA	CHA-C1A-NA	-2.28	121.18	126.40
31	n	614	CLA	CHA-C1A-NA	-2.28	121.18	126.40
31	n	603	CLA	O2A-CGA-CBA	2.28	119.06	111.91
31	B1	614	CLA	CMB-C2B-C3B	2.28	128.94	124.68
31	N	602	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
31	b	612	CLA	CHA-C1A-NA	-2.28	121.18	126.40
31	s	603	CLA	CHA-C1A-NA	-2.28	121.18	126.40
31	N	610	CLA	O1D-CGD-CBD	-2.28	119.83	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A1	407	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
31	c1	509	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
31	Y1	613	CLA	CMB-C2B-C3B	2.28	128.94	124.68
31	c	506	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
31	R1	610	CLA	O2A-CGA-CBA	2.28	119.05	111.91
49	N	622	XAT	C39-C29-C30	-2.28	119.73	122.92
31	c	505	CLA	CHD-C1D-ND	-2.28	122.36	124.45
31	b1	614	CLA	CHA-C1A-NA	-2.28	121.19	126.40
31	b1	616	CLA	CHA-C1A-NA	-2.28	121.19	126.40
31	C1	512	CLA	C1D-ND-C4D	-2.28	104.72	106.33
33	C1	514	BCR	C40-C30-C25	-2.28	106.61	110.30
47	N1	609	CHL	CMB-C2B-C1B	-2.28	124.97	128.46
31	B1	607	CLA	CHA-C1A-NA	-2.28	121.19	126.40
31	r	612	CLA	C1-C2-C3	-2.28	122.11	126.04
31	r	602	CLA	O2A-CGA-CBA	2.28	119.05	111.91
31	R	612	CLA	CMA-C3A-C4A	2.28	117.89	111.77
31	C	506	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
47	N	607	CHL	CMB-C2B-C1B	-2.28	124.97	128.46
31	Y	604	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
34	a1	412	SQD	O3-C3-C2	-2.27	105.09	110.35
47	y1	607	CHL	CMB-C2B-C1B	-2.27	124.97	128.46
31	C1	512	CLA	CHA-C1A-NA	-2.27	121.19	126.40
31	R1	610	CLA	CHA-C4D-ND	2.27	137.26	132.50
32	A1	409	PHO	C1-C2-C3	-2.27	122.11	126.04
50	Y	623	NEX	C20-C13-C14	-2.27	119.74	122.92
31	c	501	CLA	CMA-C3A-C4A	2.27	117.88	111.77
31	B	614	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
31	r	604	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
31	Y1	613	CLA	C2D-C1D-ND	2.27	111.78	110.10
31	y	613	CLA	O2A-CGA-CBA	2.27	119.04	111.91
31	s1	605	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
47	N1	607	CHL	CMB-C2B-C1B	-2.27	124.97	128.46
31	G	604	CLA	O2A-CGA-CBA	2.27	119.04	111.91
31	D1	403	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
41	D1	408	LHG	C5-O7-C7	-2.27	112.20	117.79
33	c	517	BCR	C35-C13-C12	2.27	121.66	118.08
31	C1	513	CLA	C1-O2A-CGA	2.27	122.41	116.44
31	b	602	CLA	C1D-ND-C4D	-2.27	104.72	106.33
31	C	511	CLA	CHA-C1A-NA	-2.27	121.20	126.40
31	b1	611	CLA	CHA-C1A-NA	-2.27	121.20	126.40
31	c	511	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
31	N1	610	CLA	CAC-C3C-C4C	2.27	127.76	124.81

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	402	CLA	CHA-C4D-ND	2.27	137.25	132.50
31	B1	602	CLA	CMA-C3A-C4A	2.27	117.88	111.77
31	G1	604	CLA	CHA-C1A-NA	-2.27	121.20	126.40
47	s1	606	CHL	C1B-CHB-C4A	-2.27	125.62	130.12
31	A	410	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
47	N	609	CHL	CMB-C2B-C1B	-2.27	124.97	128.46
31	S	614	CLA	CHA-C1A-NA	-2.27	121.20	126.40
31	R	610	CLA	O2A-CGA-CBA	2.27	119.03	111.91
31	R	610	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
47	S	606	CHL	C1B-CHB-C4A	-2.27	125.62	130.12
46	H	101	RRX	C30-C25-C24	2.27	122.20	115.78
31	Y	602	CLA	CHA-C4D-ND	2.27	137.25	132.50
31	s1	610	CLA	C2D-C1D-ND	2.27	111.78	110.10
31	G1	613	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
47	n1	605	CHL	CHB-C4A-NA	2.27	127.65	124.51
49	y1	622	XAT	C39-C29-C30	-2.27	119.74	122.92
31	N1	610	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
47	N	608	CHL	CMB-C2B-C1B	-2.27	124.98	128.46
47	Y	601	CHL	C1-O2A-CGA	2.27	122.40	116.44
31	r1	612	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
50	N1	623	NEX	C31-C32-C33	2.27	132.79	126.42
47	n	601	CHL	C1-O2A-CGA	2.27	122.39	116.44
31	B1	603	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
31	G	611	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
31	n	603	CLA	C1D-ND-C4D	-2.27	104.72	106.33
31	c1	507	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
31	n1	614	CLA	CHA-C1A-NA	-2.27	121.20	126.40
31	C	512	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
31	b	617	CLA	CHA-C1A-NA	-2.27	121.21	126.40
47	N	608	CHL	C4D-CHA-C1A	2.27	124.01	121.25
47	g	601	CHL	C4D-CHA-C1A	2.27	124.01	121.25
48	R1	620	LUT	C1-C6-C7	2.27	122.19	115.78
31	B	609	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
31	C	509	CLA	CHA-C1A-NA	-2.27	121.21	126.40
50	s	623	NEX	C4-C3-C2	2.27	115.15	110.77
47	Y1	601	CHL	C1-O2A-CGA	2.27	122.39	116.44
31	A	407	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
46	h	101	RRX	C16-C17-C18	-2.27	124.08	127.31
31	Y	612	CLA	CHA-C4D-ND	2.27	137.24	132.50
31	N	613	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
33	b	618	BCR	C32-C1-C6	-2.27	106.62	110.30
47	G	609	CHL	CMA-C3A-C4A	2.27	117.86	111.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	h	101	RRX	C20-C21-C22	-2.27	124.08	127.31
31	B	603	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
41	D1	408	LHG	O8-C23-C24	2.27	119.02	111.91
31	D	402	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
31	Y1	604	CLA	O2A-CGA-CBA	2.26	119.02	111.91
31	a1	406	CLA	CMD-C2D-C3D	-2.26	122.40	127.61
49	y	622	XAT	C19-C9-C10	-2.26	119.75	122.92
50	r1	622	NEX	C1-C2-C3	2.26	118.76	113.64
47	S1	606	CHL	C1B-CHB-C4A	-2.26	125.63	130.12
47	S	607	CHL	C4D-CHA-C1A	2.26	124.00	121.25
31	C	503	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
31	C1	506	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
31	r1	608	CLA	CHA-C1A-NA	-2.26	121.21	126.40
31	S	613	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
31	b	608	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
31	A	405	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
48	G	620	LUT	C38-C25-C24	-2.26	118.72	123.56
31	y1	614	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
31	g	611	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
31	C	512	CLA	CMA-C3A-C4A	2.26	117.85	111.77
47	G1	607	CHL	C4A-NA-C1A	2.26	107.72	106.71
31	g1	614	CLA	C1-O2A-CGA	2.26	122.38	116.44
31	B1	602	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
31	s	603	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
31	n1	613	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
33	c	514	BCR	C30-C25-C26	-2.26	119.43	122.61
50	Y	623	NEX	C31-C32-C33	2.26	132.77	126.42
47	y1	609	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
31	y1	614	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
31	N1	604	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
47	Y	601	CHL	CMB-C2B-C1B	-2.26	124.99	128.46
49	g	622	XAT	C20-C13-C14	-2.26	119.76	122.92
31	N	604	CLA	O2A-CGA-CBA	2.26	119.00	111.91
31	Y1	603	CLA	O2A-CGA-CBA	2.26	119.00	111.91
31	N	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	B	616	CLA	CMA-C3A-C4A	2.26	117.85	111.77
31	B1	605	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
47	S1	608	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
31	S	603	CLA	O2A-CGA-CBA	2.26	119.00	111.91
31	s	604	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
31	B	603	CLA	O2A-CGA-CBA	2.26	119.00	111.91
50	r1	622	NEX	C26-C27-C28	-2.26	121.22	125.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	610	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
31	b1	608	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	b	611	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
47	R1	607	CHL	CHB-C4A-NA	2.26	127.64	124.51
31	C	504	CLA	CHA-C4D-ND	2.26	137.22	132.50
31	y1	611	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
50	S	622	NEX	C20-C13-C14	-2.26	119.76	122.92
31	S	609	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	B	605	CLA	O2A-CGA-CBA	2.26	118.99	111.91
49	R	621	XAT	O24-C25-C24	2.26	115.08	113.38
47	s	606	CHL	C4A-NA-C1A	2.26	107.72	106.71
31	R1	603	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	C1	502	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
31	b1	612	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
33	a1	411	BCR	C35-C13-C12	2.26	121.63	118.08
31	r1	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	B1	603	CLA	O2A-CGA-CBA	2.26	118.99	111.91
50	g1	623	NEX	C31-C32-C33	2.26	132.75	126.42
33	b1	619	BCR	C36-C18-C17	-2.26	119.76	122.92
31	s	613	CLA	CHD-C1D-ND	-2.26	122.38	124.45
31	n1	610	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
34	B1	621	SQD	O3-C3-C2	-2.26	105.14	110.35
31	c1	507	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
50	N1	623	NEX	C19-C9-C10	-2.26	119.76	122.92
33	b	619	BCR	C8-C7-C6	-2.25	120.87	127.20
48	s1	620	LUT	C1-C6-C5	-2.25	119.44	122.61
47	g1	606	CHL	CAA-C2A-C3A	-2.25	106.60	112.78
31	y	612	CLA	CHA-C1A-NA	-2.25	121.23	126.40
33	A1	411	BCR	C36-C18-C17	-2.25	119.77	122.92
31	C	508	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
31	B1	616	CLA	CHA-C1A-NA	-2.25	121.24	126.40
31	n	614	CLA	C1D-ND-C4D	-2.25	104.73	106.33
31	c	513	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
31	n	604	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
31	N	612	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
31	s	602	CLA	C2C-C1C-NC	2.25	112.08	109.97
31	B	604	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
31	B	613	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
31	c1	513	CLA	C1D-ND-C4D	-2.25	104.73	106.33
37	B	620	C7Z	C18-C5-C4	2.25	118.53	114.36
47	Y	609	CHL	CHD-C4C-C3C	2.25	128.15	124.84
31	s1	609	CLA	CHA-C1A-NA	-2.25	121.24	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	604	CLA	O2A-CGA-CBA	2.25	118.97	111.91
48	n	621	LUT	C1-C6-C5	-2.25	119.44	122.61
31	G	610	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
31	B1	612	CLA	CHA-C4D-ND	2.25	137.21	132.50
33	C1	517	BCR	C34-C9-C10	-2.25	119.77	122.92
47	N1	606	CHL	C1-O2A-CGA	2.25	122.35	116.44
31	r	610	CLA	CHA-C1A-NA	-2.25	121.24	126.40
31	r	613	CLA	CHA-C1A-NA	-2.25	121.24	126.40
31	s1	602	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
49	n	622	XAT	C40-C33-C34	-2.25	119.77	122.92
49	r1	621	XAT	C19-C9-C10	-2.25	119.77	122.92
31	R1	609	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
31	n	613	CLA	CHA-C4D-ND	2.25	137.21	132.50
34	c	626	SQD	O3-C3-C2	-2.25	105.15	110.35
31	R	608	CLA	CHA-C1A-NA	-2.25	121.25	126.40
31	r1	603	CLA	CMA-C3A-C4A	2.25	117.82	111.77
31	A1	407	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
31	A1	410	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
47	n	609	CHL	C4D-CHA-C1A	2.25	123.99	121.25
34	b1	621	SQD	O3-C3-C2	-2.25	105.15	110.35
31	s1	610	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
31	B	617	CLA	CHA-C1A-NA	-2.25	121.25	126.40
47	y	601	CHL	CMB-C2B-C1B	-2.25	125.01	128.46
31	y	603	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
31	R1	612	CLA	CHA-C1A-NA	-2.25	121.25	126.40
31	R	611	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
41	g	624	LHG	C5-O7-C7	-2.25	112.25	117.79
31	c	506	CLA	C1-C2-C3	-2.25	122.15	126.04
31	G1	613	CLA	O2A-CGA-CBA	2.25	118.96	111.91
48	Y1	620	LUT	C31-C32-C33	-2.25	120.10	126.42
31	b1	607	CLA	C1D-ND-C4D	-2.25	104.74	106.33
31	b1	617	CLA	C1-O2A-CGA	2.25	122.34	116.44
31	C	512	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
31	R	613	CLA	CHA-C1A-NA	-2.25	121.25	126.40
31	C	509	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
47	S	606	CHL	C4D-CHA-C1A	2.25	123.98	121.25
48	g	621	LUT	C40-C33-C34	-2.25	119.78	122.92
31	b	610	CLA	C1-O2A-CGA	2.25	122.34	116.44
33	c	514	BCR	C37-C22-C21	-2.25	119.78	122.92
31	N1	611	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
31	c	507	CLA	O2A-CGA-CBA	2.25	118.96	111.91
31	Y1	612	CLA	CHA-C1A-NA	-2.25	121.25	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	613	CLA	O2A-CGA-CBA	2.25	118.96	111.91
31	b1	614	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
31	N	602	CLA	CMB-C2B-C3B	2.25	128.88	124.68
31	n	612	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
31	y	604	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
31	Y1	610	CLA	CHA-C4D-ND	2.25	137.20	132.50
31	c1	502	CLA	C11-C12-C13	-2.25	108.66	115.92
31	C	506	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
31	N1	604	CLA	OBD-CAD-C3D	-2.25	123.12	128.52
31	g	614	CLA	C1-O2A-CGA	2.24	122.33	116.44
47	G	601	CHL	CHD-C4C-C3C	2.24	128.14	124.84
47	n1	609	CHL	CHD-C4C-C3C	2.24	128.14	124.84
31	C1	506	CLA	O2A-CGA-CBA	2.24	118.95	111.91
31	s1	617	CLA	CAA-C2A-C3A	-2.24	106.63	112.78
31	s1	603	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	S	605	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	S	602	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
31	c1	509	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
31	G	612	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	C	507	CLA	O2A-CGA-CBA	2.24	118.94	111.91
31	B	604	CLA	CMC-C2C-C1C	2.24	128.45	125.04
31	n1	614	CLA	C1D-ND-C4D	-2.24	104.74	106.33
31	C	505	CLA	C1-C2-C3	-2.24	122.17	126.04
31	G1	602	CLA	CMB-C2B-C3B	2.24	128.87	124.68
47	n	608	CHL	CMB-C2B-C1B	-2.24	125.02	128.46
31	S1	614	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	Y	602	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
31	s1	617	CLA	CMB-C2B-C3B	2.24	128.87	124.68
31	s1	617	CLA	CHA-C1A-NA	-2.24	121.27	126.40
31	b	614	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
31	s1	604	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
31	c	510	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
31	g1	613	CLA	C1D-ND-C4D	-2.24	104.74	106.33
31	c	503	CLA	CHA-C1A-NA	-2.24	121.27	126.40
31	B1	614	CLA	CHA-C1A-NA	-2.24	121.27	126.40
31	s1	604	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
50	N1	623	NEX	C40-C33-C34	-2.24	119.78	122.92
31	c	512	CLA	CHA-C1A-NA	-2.24	121.27	126.40
31	b1	604	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
47	Y	609	CHL	CHB-C4A-NA	2.24	127.61	124.51
31	s	611	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
31	y1	613	CLA	O2D-CGD-O1D	-2.24	119.46	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	n1	608	CHL	CMB-C2B-C1B	-2.24	125.02	128.46
48	S	621	LUT	C18-C5-C4	2.24	118.50	114.36
31	B1	611	CLA	C1-C2-C3	-2.24	122.17	126.04
31	A1	407	CLA	O2A-CGA-CBA	2.24	118.94	111.91
31	y	614	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
31	G	613	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
31	b	605	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
47	y	601	CHL	C1-C2-C3	-2.24	122.17	126.04
31	g	611	CLA	CHA-C1A-NA	-2.24	121.27	126.40
31	b1	614	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
53	y	625	SPH	C3-C4-C5	-2.24	119.80	124.79
31	C1	505	CLA	C2D-C1D-ND	2.24	111.75	110.10
50	y	623	NEX	C11-C12-C13	2.24	132.70	126.42
31	s	617	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
33	C	515	BCR	C36-C18-C17	-2.24	119.79	122.92
50	y1	623	NEX	C20-C13-C14	-2.24	119.79	122.92
48	s	621	LUT	C8-C7-C6	-2.24	120.92	127.20
31	g	612	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
31	Y	610	CLA	C1D-ND-C4D	-2.24	104.75	106.33
40	C1	520	DGD	O6D-C5D-C6D	2.24	111.18	106.67
31	B1	606	CLA	C2D-C1D-ND	2.24	111.75	110.10
31	a1	405	CLA	C1-O2A-CGA	2.24	122.31	116.44
31	R1	612	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
47	G	605	CHL	C1B-CHB-C4A	-2.24	125.69	130.12
31	c	502	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
31	R1	609	CLA	C1D-ND-C4D	-2.24	104.75	106.33
33	c1	517	BCR	C1-C6-C7	2.24	122.10	115.78
31	B1	605	CLA	CMA-C3A-C2A	2.24	122.84	113.83
31	c	512	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
31	c	507	CLA	C1-O2A-CGA	2.24	122.31	116.44
56	r1	626	ERG	C15-C14-C13	2.23	106.20	104.21
31	y	608	CLA	CHA-C1A-NA	-2.23	121.28	126.40
45	F1	101	HEM	C4D-ND-C1D	2.23	107.38	105.07
31	G	610	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
31	b1	617	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
31	g1	603	CLA	CHA-C1A-NA	-2.23	121.28	126.40
31	d	402	CLA	CAC-C3C-C4C	2.23	127.71	124.81
31	n	613	CLA	CMB-C2B-C3B	2.23	128.86	124.68
31	b	603	CLA	C1D-ND-C4D	-2.23	104.75	106.33
31	c1	504	CLA	C1D-ND-C4D	-2.23	104.75	106.33
31	Y	612	CLA	CHA-C1A-NA	-2.23	121.28	126.40
44	d	405	PL9	O1-C4-C3	-2.23	118.26	120.72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y1	608	CLA	CHA-C1A-NA	-2.23	121.28	126.40
47	Y	606	CHL	C4A-NA-C1A	2.23	107.71	106.71
31	S1	604	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	c	503	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
31	C1	511	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
31	B	606	CLA	CHA-C1A-NA	-2.23	121.28	126.40
31	S	612	CLA	CHA-C1A-NA	-2.23	121.28	126.40
31	n1	602	CLA	C1D-ND-C4D	-2.23	104.75	106.33
31	B	609	CLA	C1-O2A-CGA	2.23	122.30	116.44
31	C1	503	CLA	CHA-C1A-NA	-2.23	121.29	126.40
31	Y	614	CLA	O2A-CGA-CBA	2.23	118.91	111.91
33	D	404	BCR	C33-C5-C6	-2.23	122.02	124.53
31	c1	507	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	Y1	602	CLA	CHA-C1A-NA	-2.23	121.29	126.40
47	y1	607	CHL	C1-C2-C3	-2.23	122.18	126.04
33	C1	516	BCR	C31-C1-C6	-2.23	106.68	110.30
34	C1	526	SQD	O3-C3-C2	-2.23	105.19	110.35
31	y	610	CLA	CHA-C1A-NA	-2.23	121.29	126.40
48	s	621	LUT	C1-C6-C7	2.23	122.09	115.78
31	G1	603	CLA	O2A-CGA-CBA	2.23	118.91	111.91
31	n	612	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	C1	510	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
31	s1	612	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
31	Y	604	CLA	C1D-ND-C4D	-2.23	104.75	106.33
47	g	606	CHL	CMB-C2B-C1B	-2.23	125.04	128.46
31	c	507	CLA	C1-C2-C3	-2.23	122.19	126.04
33	b	618	BCR	C34-C9-C10	-2.23	119.80	122.92
31	s	604	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
31	B	608	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
31	b1	615	CLA	O2A-CGA-CBA	2.23	118.90	111.91
31	B1	614	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
41	G	630	LHG	C6-C5-C4	-2.23	106.52	111.79
31	C1	504	CLA	C1-O2A-CGA	2.23	122.29	116.44
31	n1	611	CLA	O2A-CGA-CBA	2.23	118.90	111.91
31	C1	508	CLA	C2C-C1C-NC	2.23	112.06	109.97
31	r	608	CLA	CHA-C1A-NA	-2.23	121.30	126.40
47	Y	606	CHL	C4D-CHA-C1A	2.23	123.96	121.25
31	S1	611	CLA	C2D-C1D-ND	2.23	111.75	110.10
31	g	613	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
31	N1	604	CLA	CMB-C2B-C3B	2.23	128.84	124.68
31	R	604	CLA	CMA-C3A-C4A	2.23	117.76	111.77
31	S1	605	CLA	CHA-C1A-NA	-2.23	121.30	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	513	CLA	C1-C2-C3	-2.23	122.19	126.04
33	D1	404	BCR	C37-C22-C21	-2.23	119.81	122.92
47	N	609	CHL	C4D-CHA-C1A	2.23	123.96	121.25
31	S	602	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
31	b	603	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
31	B	607	CLA	CHA-C1A-NA	-2.22	121.30	126.40
31	N	611	CLA	O2A-CGA-CBA	2.22	118.89	111.91
31	Y1	612	CLA	C1-C2-C3	-2.22	122.20	126.04
49	g1	622	XAT	C20-C13-C14	-2.22	119.81	122.92
34	B1	626	SQD	O3-C3-C2	-2.22	105.21	110.35
47	N	608	CHL	C1B-CHB-C4A	-2.22	125.71	130.12
48	y	620	LUT	C30-C31-C32	-2.22	116.28	123.22
32	A	408	PHO	O2A-CGA-O1A	-2.22	117.98	123.59
31	R	603	CLA	O2A-CGA-CBA	2.22	118.88	111.91
31	R	602	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
31	G	614	CLA	C1D-ND-C4D	-2.22	104.76	106.33
31	C	510	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
37	b	620	C7Z	C19-C9-C10	-2.22	119.81	122.92
33	b1	619	BCR	C8-C7-C6	-2.22	120.96	127.20
31	r	603	CLA	O2A-CGA-CBA	2.22	118.88	111.91
31	c1	504	CLA	O2A-CGA-CBA	2.22	118.88	111.91
50	N1	623	NEX	C26-C27-C28	-2.22	121.30	125.99
31	Y1	614	CLA	CHA-C1A-NA	-2.22	121.31	126.40
50	G1	623	NEX	C31-C32-C33	2.22	132.65	126.42
31	b	609	CLA	CHA-C1A-NA	-2.22	121.31	126.40
31	B	610	CLA	O2A-CGA-CBA	2.22	118.88	111.91
31	R	613	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
31	N	610	CLA	C1D-ND-C4D	-2.22	104.76	106.33
47	N	606	CHL	C4A-NA-C1A	2.22	107.70	106.71
31	B1	611	CLA	C1-O2A-CGA	2.22	122.27	116.44
31	B1	616	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
31	b	602	CLA	O2A-CGA-CBA	2.22	118.87	111.91
31	b	613	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
44	d1	405	PL9	O2-C1-C6	2.22	124.43	120.59
31	B	611	CLA	CHA-C1A-NA	-2.22	121.32	126.40
31	C1	510	CLA	C2D-C1D-ND	2.22	111.74	110.10
31	R	612	CLA	OBD-CAD-C3D	-2.22	123.18	128.52
31	a1	405	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
47	N1	606	CHL	CMA-C3A-C4A	2.22	117.73	111.77
31	b1	612	CLA	CMB-C2B-C1B	-2.22	125.06	128.46
47	G1	609	CHL	CHD-C4C-C3C	2.22	128.10	124.84
31	Y	611	CLA	CMD-C2D-C3D	-2.22	122.51	127.61

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	616	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
31	R	611	CLA	C1D-ND-C4D	-2.22	104.76	106.33
31	B	604	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
31	Y	611	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
31	S1	602	CLA	C1-C2-C3	-2.22	122.21	126.04
31	n1	614	CLA	C1-O2A-CGA	2.22	122.26	116.44
48	n	621	LUT	C19-C9-C10	-2.22	119.82	122.92
31	n	612	CLA	CHA-C4D-ND	2.22	137.13	132.50
31	n1	604	CLA	CMA-C3A-C4A	2.22	117.73	111.77
31	B	605	CLA	CHA-C1A-NA	-2.22	121.32	126.40
31	n1	612	CLA	CHA-C1A-NA	-2.22	121.32	126.40
47	G1	605	CHL	C4A-NA-C1A	2.22	107.70	106.71
48	n	621	LUT	C35-C34-C33	-2.21	124.15	127.31
31	n1	604	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
31	n1	610	CLA	CHA-C1A-NA	-2.21	121.33	126.40
34	b	621	SQD	O3-C3-C2	-2.21	105.23	110.35
31	b	611	CLA	O2A-CGA-CBA	2.21	118.86	111.91
31	c	503	CLA	O2A-CGA-CBA	2.21	118.86	111.91
31	B	617	CLA	OBD-CAD-C3D	-2.21	123.19	128.52
31	C	505	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
48	N	621	LUT	C31-C30-C29	-2.21	124.15	127.31
31	Y1	614	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
31	c1	508	CLA	CHA-C4D-ND	2.21	137.13	132.50
31	y	610	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
31	Y1	603	CLA	CHA-C1A-NA	-2.21	121.33	126.40
47	Y	607	CHL	C4A-NA-C1A	2.21	107.70	106.71
47	G1	607	CHL	C3C-C4C-NC	-2.21	108.09	110.57
31	C	513	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
31	n	611	CLA	C1D-ND-C4D	-2.21	104.76	106.33
31	N1	612	CLA	C1D-ND-C4D	-2.21	104.76	106.33
47	r1	606	CHL	CMB-C2B-C1B	-2.21	125.06	128.46
31	r1	610	CLA	CHA-C1A-NA	-2.21	121.33	126.40
49	N	622	XAT	C19-C9-C10	-2.21	119.82	122.92
33	C1	514	BCR	C19-C18-C17	2.21	122.33	118.94
31	s1	609	CLA	CMB-C2B-C3B	2.21	128.82	124.68
49	Y	622	XAT	C39-C29-C30	-2.21	119.83	122.92
31	b	603	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	B1	610	CLA	CMA-C3A-C4A	2.21	117.72	111.77
31	C	503	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	B	603	CLA	CHA-C1A-NA	-2.21	121.33	126.40
31	a1	405	CLA	CHA-C1A-NA	-2.21	121.33	126.40
31	G	603	CLA	CAA-C2A-C3A	-2.21	106.72	112.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	G1	606	CHL	C1-O2A-CGA	2.21	122.24	116.44
31	G	611	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	G1	612	CLA	CHD-C1D-ND	-2.21	122.42	124.45
31	Y	612	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	S1	603	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	g1	603	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
47	y	606	CHL	C4D-CHA-C1A	2.21	123.94	121.25
31	b1	617	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
33	b1	618	BCR	C36-C18-C17	-2.21	119.83	122.92
31	r1	610	CLA	O2A-CGA-CBA	2.21	118.84	111.91
31	g	614	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
34	B	621	SQD	O3-C3-C2	-2.21	105.24	110.35
31	B	612	CLA	CHA-C1A-NA	-2.21	121.34	126.40
31	G1	610	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
31	Y	604	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
31	A	406	CLA	O2A-CGA-CBA	2.21	118.84	111.91
31	G1	610	CLA	CHA-C4D-ND	2.21	137.12	132.50
31	b	614	CLA	O2A-CGA-CBA	2.21	118.83	111.91
31	y1	612	CLA	CHA-C1A-NA	-2.21	121.34	126.40
31	r1	604	CLA	O2A-CGA-CBA	2.21	118.83	111.91
31	s1	609	CLA	O2A-CGA-CBA	2.21	118.83	111.91
31	g	603	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
35	D	411	LMG	O6-C5-C6	2.21	111.92	106.44
31	G1	603	CLA	CHA-C1A-NA	-2.21	121.34	126.40
31	y1	610	CLA	CHA-C1A-NA	-2.21	121.34	126.40
33	c1	514	BCR	C4-C5-C6	-2.21	119.53	122.73
31	s1	612	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
31	C1	508	CLA	CHA-C4D-ND	2.21	137.11	132.50
31	b1	609	CLA	C1-O2A-CGA	2.21	122.23	116.44
31	d	402	CLA	O2A-CGA-CBA	2.21	118.83	111.91
31	N1	613	CLA	CHA-C1A-NA	-2.21	121.35	126.40
31	C1	512	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
33	d	404	BCR	C35-C13-C12	2.20	121.55	118.08
31	Y1	614	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
31	Y1	612	CLA	C1D-ND-C4D	-2.20	104.77	106.33
33	c	515	BCR	C1-C6-C7	2.20	122.01	115.78
31	b	611	CLA	CHA-C1A-NA	-2.20	121.35	126.40
31	B1	604	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
31	a1	406	CLA	O2A-CGA-CBA	2.20	118.82	111.91
35	b1	622	LMG	C9-C8-C7	-2.20	106.58	111.79
31	B1	605	CLA	C1D-ND-C4D	-2.20	104.77	106.33
31	c1	501	CLA	C1D-ND-C4D	-2.20	104.77	106.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c1	503	CLA	C1D-ND-C4D	-2.20	104.77	106.33
31	S	610	CLA	CHA-C1A-NA	-2.20	121.35	126.40
47	n	605	CHL	CHD-C4C-C3C	2.20	128.08	124.84
44	d	405	PL9	C27-C28-C29	-2.20	122.36	127.66
31	R	603	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	R1	609	CLA	CMB-C2B-C3B	2.20	128.80	124.68
31	S	617	CLA	CHA-C1A-NA	-2.20	121.35	126.40
31	b1	603	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	y1	610	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
31	C1	511	CLA	CHA-C1A-NA	-2.20	121.36	126.40
37	B1	620	C7Z	C2-C3-C4	2.20	113.32	110.30
31	b1	610	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
47	G	606	CHL	C1B-CHB-C4A	-2.20	125.76	130.12
50	Y1	623	NEX	C26-C27-C28	-2.20	121.34	125.99
31	B1	604	CLA	C1D-ND-C4D	-2.20	104.77	106.33
31	B1	602	CLA	O2A-CGA-CBA	2.20	118.82	111.91
47	s	608	CHL	CHB-C4A-NA	2.20	127.56	124.51
47	G	607	CHL	CMA-C3A-C4A	2.20	117.69	111.77
31	b1	615	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
49	Y1	622	XAT	C40-C33-C34	-2.20	119.84	122.92
31	s1	610	CLA	CHA-C1A-NA	-2.20	121.36	126.40
47	y	609	CHL	C1B-CHB-C4A	-2.20	125.76	130.12
47	R1	606	CHL	C3C-C4C-NC	-2.20	108.10	110.57
31	N1	612	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	N1	603	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
31	R1	610	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
31	c1	509	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
31	C	513	CLA	C1D-ND-C4D	-2.20	104.77	106.33
31	B	616	CLA	C2A-C1A-CHA	2.20	127.71	123.86
31	g1	602	CLA	CMB-C2B-C3B	2.20	128.79	124.68
31	B	609	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	Y1	611	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	A1	405	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
31	Y	610	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
31	B	609	CLA	C2D-C1D-ND	2.20	111.72	110.10
48	s	621	LUT	C10-C11-C12	-2.20	116.35	123.22
46	H1	101	RRX	C37-C22-C21	-2.20	119.84	122.92
31	S1	609	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	y	603	CLA	O2A-CGA-CBA	2.20	118.81	111.91
31	S	611	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	c	506	CLA	C1-O2A-CGA	2.20	122.21	116.44
35	B1	622	LMG	O7-C10-O9	-2.20	118.39	123.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	G	621	LUT	C35-C15-C14	-2.20	118.97	123.47
31	c	505	CLA	C1-O2A-CGA	2.20	122.21	116.44
47	Y	607	CHL	C1B-CHB-C4A	-2.20	125.76	130.12
31	n1	604	CLA	CHA-C1A-NA	-2.20	121.36	126.40
48	g1	621	LUT	C31-C32-C33	-2.20	120.24	126.42
31	G1	610	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
31	s1	613	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
31	n1	610	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
31	B1	617	CLA	C1C-C2C-C3C	-2.20	104.65	106.96
31	C1	508	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
31	n1	610	CLA	CMA-C3A-C4A	2.20	117.68	111.77
44	D	405	PL9	C31-C32-C33	-2.20	104.66	111.88
31	Y1	604	CLA	C6-C7-C8	-2.20	108.82	115.92
33	c1	515	BCR	C38-C26-C25	-2.20	122.06	124.53
47	N1	606	CHL	C1-C2-C3	-2.20	122.25	126.04
31	n1	611	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
31	C	506	CLA	O2A-CGA-CBA	2.20	118.80	111.91
31	S1	611	CLA	CHA-C1A-NA	-2.20	121.37	126.40
31	C	511	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
31	n1	610	CLA	C2A-C1A-CHA	2.19	127.70	123.86
31	S1	613	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
47	n1	605	CHL	C4D-CHA-C1A	2.19	123.92	121.25
49	g	622	XAT	C40-C33-C34	-2.19	119.85	122.92
50	n1	623	NEX	C28-C29-C30	2.19	122.31	118.94
31	S1	602	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	s	609	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
31	B	606	CLA	CMA-C3A-C4A	2.19	117.67	111.77
31	Y	604	CLA	CMA-C3A-C4A	2.19	117.67	111.77
31	N	612	CLA	CHA-C1A-NA	-2.19	121.38	126.40
31	b	607	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
47	g	608	CHL	C1B-CHB-C4A	-2.19	125.77	130.12
47	y	605	CHL	C4D-CHA-C1A	2.19	123.92	121.25
31	B	602	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
31	c1	503	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
31	a1	405	CLA	O2A-CGA-CBA	2.19	118.78	111.91
47	Y	609	CHL	CMB-C2B-C1B	-2.19	125.10	128.46
44	D	405	PL9	O1-C4-C3	-2.19	118.31	120.72
31	b	612	CLA	CHA-C4D-ND	2.19	137.08	132.50
31	A1	405	CLA	C6-C5-C3	-2.19	107.71	113.45
31	B1	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	n	604	CLA	C1D-ND-C4D	-2.19	104.78	106.33
33	B1	618	BCR	C19-C18-C17	2.19	122.30	118.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D1	402	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	G1	603	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	d1	403	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	y	604	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
31	R1	608	CLA	CHA-C1A-NA	-2.19	121.38	126.40
31	g1	614	CLA	CHA-C1A-NA	-2.19	121.38	126.40
48	r1	620	LUT	C11-C12-C13	-2.19	120.27	126.42
33	c1	515	BCR	C15-C14-C13	-2.19	124.19	127.31
31	B	611	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	a1	407	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
50	R	622	NEX	O24-C25-C24	-2.19	111.74	113.38
31	r1	603	CLA	C1-O2A-CGA	2.19	122.19	116.44
31	b	614	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	r	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
47	G	605	CHL	C1-O2A-CGA	2.19	123.09	116.73
56	R1	626	ERG	C1-C10-C9	-2.19	103.75	108.28
31	Y	604	CLA	O2A-CGA-CBA	2.19	118.77	111.91
31	C1	510	CLA	O2A-CGA-CBA	2.19	118.77	111.91
31	B	611	CLA	CMB-C2B-C3B	2.19	128.77	124.68
31	b1	603	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	c1	512	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	g1	610	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	g	604	CLA	C1D-ND-C4D	-2.19	104.78	106.33
31	n1	603	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	Y1	614	CLA	C2D-C1D-ND	2.19	111.72	110.10
31	B1	614	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
33	a1	411	BCR	C37-C22-C23	2.19	121.52	118.08
31	Y	614	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	c1	502	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
31	r	612	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
47	n1	609	CHL	CHB-C4A-NA	2.19	127.53	124.51
48	R1	620	LUT	C31-C32-C33	-2.19	120.28	126.42
31	n	612	CLA	CMB-C2B-C3B	2.19	128.77	124.68
31	a1	410	CLA	CMD-C2D-C3D	-2.19	122.59	127.61
46	H	101	RRX	C35-C13-C14	-2.19	119.86	122.92
31	A	405	CLA	C2D-C1D-ND	2.18	111.71	110.10
31	a1	405	CLA	CMB-C2B-C3B	2.18	128.76	124.68
33	c1	517	BCR	C23-C22-C21	2.18	122.29	118.94
31	s	612	CLA	CMB-C2B-C3B	2.18	128.76	124.68
31	y1	612	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
31	c	512	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
47	G	605	CHL	C4D-CHA-C1A	2.18	123.91	121.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	605	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
31	d	402	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
31	b	612	CLA	O2A-CGA-CBA	2.18	118.76	111.91
31	R1	609	CLA	CHA-C1A-NA	-2.18	121.40	126.40
33	b	619	BCR	C15-C14-C13	-2.18	124.19	127.31
44	D1	405	PL9	C40-C39-C41	2.18	118.94	115.27
31	y1	604	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
31	b	604	CLA	C1-C2-C3	-2.18	122.27	126.04
47	y	605	CHL	C4A-NA-C1A	2.18	107.69	106.71
31	R	603	CLA	CHA-C1A-NA	-2.18	121.40	126.40
33	C	514	BCR	C38-C26-C25	-2.18	122.08	124.53
33	D1	404	BCR	C33-C5-C4	2.18	117.81	113.62
50	Y	623	NEX	C1-C2-C3	2.18	118.57	113.64
33	B	619	BCR	C31-C1-C6	-2.18	106.76	110.30
31	N	610	CLA	CMB-C2B-C3B	2.18	128.76	124.68
31	a	407	CLA	CHA-C1A-NA	-2.18	121.40	126.40
31	s1	604	CLA	CHA-C1A-NA	-2.18	121.40	126.40
31	S	610	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
31	A1	407	CLA	CHA-C1A-NA	-2.18	121.40	126.40
31	C1	507	CLA	CHA-C1A-NA	-2.18	121.40	126.40
44	D	405	PL9	C27-C28-C29	-2.18	122.41	127.66
47	g	605	CHL	C4A-NA-C1A	2.18	107.69	106.71
31	Y	603	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
31	c1	502	CLA	C11-C10-C8	-2.18	108.88	115.92
32	A1	408	PHO	C1B-NB-C4B	2.18	111.57	107.09
47	g1	605	CHL	C1B-CHB-C4A	-2.18	125.80	130.12
49	g1	622	XAT	C40-C33-C34	-2.18	119.87	122.92
37	b	620	C7Z	C4-C5-C6	-2.18	115.99	120.85
31	C	504	CLA	CMB-C2B-C3B	2.18	128.75	124.68
31	b	613	CLA	CHD-C1D-ND	-2.18	122.45	124.45
49	r1	621	XAT	C24-C23-C22	-2.18	106.57	110.77
47	g	608	CHL	C4D-CHA-C1A	2.18	123.90	121.25
50	n1	623	NEX	C20-C13-C14	-2.18	119.87	122.92
31	S1	617	CLA	C1D-ND-C4D	-2.18	104.79	106.33
31	g1	611	CLA	C1D-ND-C4D	-2.18	104.79	106.33
47	N1	606	CHL	C4A-NA-C1A	2.18	107.69	106.71
31	b	610	CLA	CHA-C1A-NA	-2.18	121.41	126.40
31	S1	617	CLA	CHA-C1A-NA	-2.18	121.41	126.40
50	g	623	NEX	C26-C27-C28	-2.18	121.39	125.99
31	r	604	CLA	CMB-C2B-C3B	2.18	128.75	124.68
49	G1	622	XAT	O4-C5-C18	-2.18	112.45	115.06
31	R1	608	CLA	C1D-ND-C4D	-2.18	104.79	106.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	604	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
35	w1	201	LMG	C8-O7-C10	-2.18	112.43	117.79
31	s	617	CLA	O2A-CGA-CBA	2.18	118.74	111.91
31	B1	614	CLA	O2A-CGA-CBA	2.18	118.74	111.91
47	n	601	CHL	C4A-NA-C1A	2.18	107.68	106.71
31	b	607	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
37	b	620	C7Z	C28-C27-C26	-2.17	121.09	127.20
31	b1	616	CLA	CMA-C3A-C4A	2.17	117.62	111.77
31	B1	615	CLA	CHA-C1A-NA	-2.17	121.42	126.40
47	y1	601	CHL	C2C-C3C-C4C	2.17	108.04	106.49
31	a1	407	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
31	Y	602	CLA	CMB-C2B-C1B	-2.17	125.12	128.46
31	R	612	CLA	CHA-C1A-NA	-2.17	121.42	126.40
31	g1	612	CLA	CHA-C1A-NA	-2.17	121.42	126.40
31	b1	609	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
47	R1	606	CHL	CMB-C2B-C1B	-2.17	125.12	128.46
31	N1	602	CLA	CHA-C4D-ND	2.17	137.05	132.50
47	S1	607	CHL	CHD-C4C-C3C	2.17	128.03	124.84
31	D	403	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
31	r	603	CLA	C1-C2-C3	-2.17	122.28	126.04
31	R1	603	CLA	CMA-C3A-C4A	2.17	117.61	111.77
31	b1	613	CLA	C2D-C1D-ND	2.17	111.70	110.10
33	D	404	BCR	C34-C9-C10	-2.17	119.88	122.92
48	g	621	LUT	C19-C9-C10	-2.17	119.88	122.92
31	C1	506	CLA	CMB-C2B-C3B	2.17	128.74	124.68
31	G	614	CLA	O2A-CGA-CBA	2.17	118.72	111.91
31	C1	507	CLA	O2A-CGA-CBA	2.17	118.72	111.91
31	b1	611	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
47	y	601	CHL	CHC-C1C-NC	2.17	127.50	124.20
37	b	620	C7Z	C2-C3-C4	2.17	113.28	110.30
48	Y1	621	LUT	C2-C3-C4	-2.17	107.33	110.30
31	y	611	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
31	y1	608	CLA	O2A-CGA-CBA	2.17	118.72	111.91
31	A1	410	CLA	CMA-C3A-C2A	2.17	122.59	113.83
31	B	611	CLA	O2A-CGA-CBA	2.17	118.72	111.91
31	n1	611	CLA	CHA-C1A-NA	-2.17	121.43	126.40
31	c1	512	CLA	CHD-C1D-ND	-2.17	122.46	124.45
50	y1	623	NEX	C31-C32-C33	2.17	132.51	126.42
31	N	613	CLA	C1D-ND-C4D	-2.17	104.79	106.33
31	A1	410	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
47	G1	601	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
31	R	604	CLA	O1D-CGD-CBD	-2.17	120.04	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Y1	607	CHL	C1-C2-C3	-2.17	122.29	126.04
31	a	407	CLA	C1-O2A-CGA	2.17	122.14	116.44
31	c1	513	CLA	C1C-C2C-C3C	-2.17	104.67	106.96
37	b1	620	C7Z	C31-C32-C33	-2.17	120.32	126.42
31	N1	613	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
31	B1	604	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
47	G1	609	CHL	C3C-C4C-NC	-2.17	108.14	110.57
56	R1	626	ERG	C16-C17-C13	2.17	106.46	103.84
31	G	603	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
31	g	602	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
49	R	621	XAT	C31-C32-C33	2.17	132.51	126.42
47	s	606	CHL	C4D-CHA-C1A	2.17	123.89	121.25
31	b1	614	CLA	CMA-C3A-C4A	2.17	117.60	111.77
31	c1	509	CLA	CMB-C2B-C3B	2.17	128.74	124.68
31	R1	602	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
31	b1	617	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
31	N	604	CLA	C1D-ND-C4D	-2.17	104.80	106.33
49	g	622	XAT	C19-C9-C8	2.17	121.49	118.08
47	G1	609	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
47	g1	609	CHL	C1-O2A-CGA	2.17	122.13	116.44
31	Y	610	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
48	R1	620	LUT	C40-C33-C34	-2.17	119.89	122.92
31	b	613	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
33	D1	404	BCR	C30-C25-C24	2.17	121.91	115.78
47	g1	608	CHL	C1B-CHB-C4A	-2.17	125.83	130.12
31	g1	602	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
31	C	508	CLA	CHA-C1A-NA	-2.17	121.44	126.40
47	Y1	607	CHL	CHD-C4C-C3C	2.17	128.02	124.84
47	g	605	CHL	C4D-CHA-C1A	2.17	123.88	121.25
31	S	602	CLA	C1D-ND-C4D	-2.17	104.80	106.33
31	S	605	CLA	C1D-ND-C4D	-2.17	104.80	106.33
31	S	609	CLA	C1D-ND-C4D	-2.17	104.80	106.33
31	B1	613	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	c1	510	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	R	611	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	B1	611	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	G1	611	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	g1	613	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	y1	603	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	G1	611	CLA	C2D-C1D-ND	2.16	111.70	110.10
31	r1	602	CLA	CMB-C2B-C3B	2.16	128.73	124.68
31	S	604	CLA	CHA-C1A-NA	-2.16	121.44	126.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	D	408	LHG	C6-C5-C4	-2.16	106.67	111.79
47	G1	605	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
31	b	605	CLA	C2D-C1D-ND	2.16	111.70	110.10
33	c1	514	BCR	C38-C26-C27	2.16	117.77	113.62
41	N	624	LHG	O7-C7-O9	-2.16	118.47	123.70
47	Y	609	CHL	C1B-CHB-C4A	-2.16	125.83	130.12
33	d1	404	BCR	C27-C26-C25	-2.16	119.59	122.73
47	g	608	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
31	r	602	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	C1	502	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	R	609	CLA	CMA-C3A-C4A	2.16	117.58	111.77
47	G1	606	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
31	a	410	CLA	CHA-C1A-NA	-2.16	121.45	126.40
48	y1	621	LUT	C10-C11-C12	-2.16	116.47	123.22
31	S	611	CLA	C2D-C1D-ND	2.16	111.70	110.10
31	B1	616	CLA	C1D-ND-C4D	-2.16	104.80	106.33
47	G	609	CHL	C1-O2A-CGA	2.16	122.11	116.44
31	B	612	CLA	O2A-CGA-CBA	2.16	118.69	111.91
46	H1	101	RRX	C8-C7-C6	-2.16	121.13	127.20
31	N1	603	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	b1	602	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
48	y	620	LUT	C20-C13-C12	2.16	121.48	118.08
31	n	612	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
49	N1	622	XAT	C20-C13-C14	-2.16	119.90	122.92
31	G	611	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	g1	604	CLA	CHA-C1A-NA	-2.16	121.45	126.40
33	c	516	BCR	C27-C26-C25	-2.16	119.59	122.73
31	S1	611	CLA	CAC-C3C-C4C	2.16	127.61	124.81
31	N	611	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
31	B1	603	CLA	C1D-ND-C4D	-2.16	104.80	106.33
31	Y	610	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
31	G	602	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
45	f1	101	HEM	C3D-C4D-ND	-2.16	107.76	110.17
31	R	602	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	B1	609	CLA	C2A-C1A-CHA	2.16	127.63	123.86
31	g	612	CLA	C1D-ND-C4D	-2.16	104.80	106.33
31	B	606	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
31	c1	507	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
32	a1	409	PHO	O2A-CGA-O1A	-2.16	118.15	123.59
47	g1	605	CHL	C1-O2A-CGA	2.16	123.00	116.73
31	c	506	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
57	Y1	627	PTY	C6-O7-C8	-2.16	113.88	117.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	602	CLA	CMB-C2B-C3B	2.16	128.71	124.68
31	A	407	CLA	CHA-C1A-NA	-2.16	121.46	126.40
31	s1	610	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
31	Y1	602	CLA	C1D-ND-C4D	-2.16	104.80	106.33
31	y1	610	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
31	B	614	CLA	O2A-CGA-CBA	2.16	118.67	111.91
33	D	404	BCR	C8-C9-C10	2.16	122.25	118.94
47	g1	601	CHL	CMB-C2B-C1B	-2.16	125.15	128.46
31	c	511	CLA	CMB-C2B-C3B	2.16	128.71	124.68
31	b1	605	CLA	CMA-C3A-C2A	2.16	122.53	113.83
47	n	608	CHL	CHD-C4C-C3C	2.16	128.01	124.84
31	G	613	CLA	CAC-C3C-C2C	-2.16	123.84	127.53
31	Y1	608	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
31	s	617	CLA	CMB-C2B-C3B	2.16	128.71	124.68
47	G	609	CHL	C4D-CHA-C1A	2.15	123.87	121.25
50	Y	623	NEX	C28-C29-C30	2.15	122.25	118.94
31	D	402	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
48	N1	620	LUT	C20-C13-C12	2.15	121.47	118.08
48	R	620	LUT	C11-C12-C13	-2.15	120.36	126.42
31	s1	614	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
31	n1	612	CLA	C1D-ND-C4D	-2.15	104.81	106.33
47	g1	601	CHL	C1B-CHB-C4A	-2.15	125.85	130.12
31	B	611	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
31	y1	608	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
31	Y1	614	CLA	O2A-CGA-CBA	2.15	118.67	111.91
31	n1	602	CLA	CHA-C1A-NA	-2.15	121.47	126.40
47	r	606	CHL	CMB-C2B-C1B	-2.15	125.15	128.46
47	N1	606	CHL	CMB-C2B-C1B	-2.15	125.15	128.46
47	Y1	606	CHL	CMB-C2B-C1B	-2.15	125.15	128.46
33	b1	619	BCR	C39-C30-C25	-2.15	106.81	110.30
31	G1	614	CLA	CHA-C1A-NA	-2.15	121.47	126.40
32	A	408	PHO	CMC-C2C-C3C	2.15	129.00	124.94
47	n	609	CHL	C1-C2-C3	-2.15	122.32	126.04
31	y	613	CLA	C1-O2A-CGA	2.15	122.09	116.44
48	R	620	LUT	C20-C13-C14	-2.15	119.91	122.92
47	G	609	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
31	G	613	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	C1	511	CLA	CMB-C2B-C3B	2.15	128.70	124.68
31	s	605	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
50	n1	623	NEX	C11-C12-C13	2.15	132.46	126.42
31	g1	611	CLA	CHA-C1A-NA	-2.15	121.47	126.40
47	Y1	605	CHL	C4A-NA-C1A	2.15	107.67	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	y	621	LUT	C31-C32-C33	-2.15	120.37	126.42
31	s	614	CLA	CHA-C1A-NA	-2.15	121.47	126.40
33	c	516	BCR	C31-C1-C6	-2.15	106.81	110.30
47	S	606	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
47	y	605	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
31	C1	501	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
50	y1	623	NEX	C40-C33-C34	-2.15	119.91	122.92
31	r1	608	CLA	O2A-CGA-CBA	2.15	118.66	111.91
48	Y	621	LUT	C10-C11-C12	-2.15	116.51	123.22
31	Y1	611	CLA	O2A-CGA-CBA	2.15	118.65	111.91
31	B1	608	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	R1	602	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	s	610	CLA	C1D-ND-C4D	-2.15	104.81	106.33
48	S	621	LUT	C1-C6-C5	-2.15	119.59	122.61
31	y	611	CLA	CHA-C1A-NA	-2.15	121.48	126.40
31	g	613	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
31	C1	505	CLA	CMA-C3A-C4A	2.15	117.55	111.77
31	s	617	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	s	611	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
48	G	620	LUT	C31-C32-C33	-2.15	120.38	126.42
44	d1	405	PL9	C31-C32-C33	-2.15	104.82	111.88
31	G	603	CLA	O2A-CGA-CBA	2.15	118.65	111.91
47	Y	605	CHL	CHD-C4C-C3C	2.15	128.00	124.84
31	n	612	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
47	R1	607	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
48	s	620	LUT	C36-C21-C22	-2.15	105.37	109.44
31	c	512	CLA	CMA-C3A-C4A	2.15	117.55	111.77
31	c	510	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
33	C1	515	BCR	C36-C18-C17	-2.15	119.92	122.92
31	G1	604	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	S1	603	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
31	c1	511	CLA	CMA-C3A-C4A	2.15	117.54	111.77
47	R	607	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
47	S	608	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
31	N	610	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	b1	607	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
47	G1	608	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
47	r1	607	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
31	s1	617	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	C	502	CLA	C1D-ND-C4D	-2.15	104.81	106.33
31	n	612	CLA	C1D-ND-C4D	-2.15	104.81	106.33
33	c	515	BCR	C35-C13-C12	2.15	121.46	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	620	C7Z	C39-C29-C30	-2.15	119.92	122.92
47	y1	609	CHL	CHD-C4C-C3C	2.15	127.99	124.84
31	Y	603	CLA	O2A-CGA-CBA	2.15	118.64	111.91
53	Y	625	SPH	C3-C4-C5	-2.14	120.01	124.79
31	C1	510	CLA	O2D-CGD-O1D	-2.14	119.64	123.84
31	s1	604	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
31	g	610	CLA	C1C-C2C-C3C	-2.14	104.70	106.96
47	S	607	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	S	609	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
31	d	403	CLA	CHA-C1A-NA	-2.14	121.49	126.40
44	d1	405	PL9	O2-C1-C2	-2.14	116.87	121.78
31	C	507	CLA	CMA-C3A-C4A	2.14	117.53	111.77
37	b	620	C7Z	C31-C32-C33	-2.14	120.39	126.42
47	N1	607	CHL	C1-C2-C3	-2.14	122.34	126.04
31	g	611	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
31	y1	604	CLA	C1D-ND-C4D	-2.14	104.81	106.33
31	B	610	CLA	C1-O2A-CGA	2.14	122.06	116.44
31	d	403	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
47	N1	606	CHL	C4D-CHA-C1A	2.14	123.86	121.25
31	N1	603	CLA	O2A-CGA-CBA	2.14	118.63	111.91
47	S1	606	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
47	y1	606	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
48	Y1	620	LUT	C31-C30-C29	-2.14	124.25	127.31
31	G	603	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	b1	604	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	C	507	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
31	B1	603	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
31	R1	612	CLA	C1-O2A-CGA	2.14	122.06	116.44
31	Y	603	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
31	b	602	CLA	CHA-C1A-NA	-2.14	121.50	126.40
49	y	622	XAT	C39-C29-C30	-2.14	119.92	122.92
47	g1	609	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	r	602	CLA	C1D-ND-C4D	-2.14	104.81	106.33
31	B1	606	CLA	CHA-C1A-NA	-2.14	121.50	126.40
32	a	409	PHO	C1-C2-C3	-2.14	122.34	126.04
40	C	519	DGD	O3G-C1D-C2D	2.14	111.64	108.30
31	B	616	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	d1	402	CLA	C1-C2-C3	-2.14	122.34	126.04
33	C1	517	BCR	C4-C5-C6	-2.14	119.63	122.73
31	G	610	CLA	CMA-C3A-C4A	2.14	117.52	111.77
47	g1	608	CHL	C4D-CHA-C1A	2.14	123.85	121.25
31	c1	508	CLA	O2D-CGD-O1D	-2.14	119.66	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	511	CLA	C1C-C2C-C3C	-2.14	104.71	106.96
33	b1	618	BCR	C1-C6-C7	2.14	121.83	115.78
47	G	606	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
31	b	615	CLA	C2A-C1A-CHA	2.14	127.60	123.86
31	s1	617	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
31	Y	613	CLA	C1D-ND-C4D	-2.14	104.82	106.33
31	s	609	CLA	C1D-ND-C4D	-2.14	104.82	106.33
47	r	607	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
44	D	405	PL9	C42-C43-C44	-2.14	122.52	127.66
31	y1	612	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
31	n	614	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
31	A1	406	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
47	Y	606	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
47	y	606	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
32	A	409	PHO	C1-C2-C3	-2.14	122.35	126.04
31	y	612	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
47	Y	601	CHL	CHC-C1C-NC	2.14	127.44	124.20
50	G1	623	NEX	C28-C29-C30	2.14	122.22	118.94
47	G	608	CHL	C1B-CHB-C4A	-2.14	125.89	130.12
31	C	501	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
47	S1	606	CHL	C4D-CHA-C1A	2.13	123.85	121.25
45	F	101	HEM	CAB-C3B-C2B	-2.13	121.57	128.60
47	N	606	CHL	CMB-C2B-C1B	-2.13	125.18	128.46
47	s	607	CHL	CMB-C2B-C1B	-2.13	125.18	128.46
33	d1	404	BCR	C33-C5-C6	-2.13	122.13	124.53
47	g	605	CHL	C1B-CHB-C4A	-2.13	125.89	130.12
31	G	602	CLA	C1D-ND-C4D	-2.13	104.82	106.33
50	S1	623	NEX	C4-C3-C2	2.13	114.89	110.77
33	c	516	BCR	C38-C26-C27	2.13	117.71	113.62
31	s1	603	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
49	n1	622	XAT	C40-C33-C34	-2.13	119.94	122.92
31	R	612	CLA	C1-C2-C3	-2.13	122.35	126.04
31	b1	609	CLA	OBD-CAD-C3D	-2.13	123.39	128.52
31	R	604	CLA	CHA-C1A-NA	-2.13	121.51	126.40
44	D1	405	PL9	C32-C33-C34	-2.13	122.53	127.66
31	g	610	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
31	c1	502	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
37	b	620	C7Z	C11-C12-C13	-2.13	120.43	126.42
31	c1	505	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	b	607	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	S1	610	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
47	S	601	CHL	CMB-C2B-C1B	-2.13	125.19	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	611	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
31	y	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	d1	402	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	G	613	CLA	C1D-ND-C4D	-2.13	104.82	106.33
31	S	604	CLA	C1D-ND-C4D	-2.13	104.82	106.33
40	C1	519	DGD	O1G-C1A-O1A	-2.13	118.21	123.59
47	s	601	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	B	608	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	B1	605	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	y	608	CLA	O2A-CGA-CBA	2.13	118.59	111.91
31	b1	614	CLA	O2A-CGA-CBA	2.13	118.59	111.91
33	C	515	BCR	C4-C5-C6	-2.13	119.64	122.73
31	G	602	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	B1	614	CLA	C1D-ND-C4D	-2.13	104.82	106.33
50	Y1	623	NEX	C4-C3-C2	2.13	114.89	110.77
31	N1	611	CLA	CMA-C3A-C4A	2.13	117.50	111.77
31	B1	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	b1	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	b	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
47	Y	601	CHL	C1B-CHB-C4A	-2.13	125.90	130.12
41	S1	624	LHG	O7-C7-O9	-2.13	118.56	123.70
47	n1	606	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
47	s1	608	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	B1	617	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
48	N	621	LUT	C20-C13-C12	2.13	121.43	118.08
47	g	601	CHL	C4A-NA-C1A	2.13	107.66	106.71
37	b1	620	C7Z	C1-C6-C7	2.13	121.80	115.78
31	g	603	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
47	Y1	607	CHL	C1-O2A-CGA	2.13	122.03	116.44
31	N	611	CLA	CHA-C1A-NA	-2.13	121.52	126.40
47	s	608	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
49	r1	621	XAT	C27-C28-C29	2.13	128.83	125.53
33	B1	618	BCR	C35-C13-C14	-2.13	119.94	122.92
31	B	609	CLA	C2A-C1A-CHA	2.13	127.58	123.86
31	B1	603	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
31	g1	603	CLA	O2A-CGA-CBA	2.13	118.58	111.91
31	y	614	CLA	CHA-C1A-NA	-2.13	121.53	126.40
47	g	609	CHL	CMA-C3A-C4A	2.13	117.49	111.77
48	g1	620	LUT	C35-C15-C14	-2.13	119.12	123.47
31	B1	604	CLA	CHA-C1A-NA	-2.13	121.53	126.40
31	c1	506	CLA	CHA-C1A-NA	-2.13	121.53	126.40
31	s1	612	CLA	CHA-C1A-NA	-2.13	121.53	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	c1	525	LHG	C6-C5-C4	-2.13	106.76	111.79
31	B	610	CLA	C1D-ND-C4D	-2.13	104.82	106.33
47	s1	607	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	s	602	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
31	y	602	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
31	g	614	CLA	CHA-C1A-NA	-2.13	121.53	126.40
47	Y	609	CHL	C4A-NA-C1A	2.13	107.66	106.71
31	Y1	613	CLA	CMC-C2C-C1C	2.13	128.28	125.04
47	g	605	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
31	g1	604	CLA	O2A-CGA-CBA	2.13	118.58	111.91
47	y1	606	CHL	CHB-C4A-NA	2.13	127.45	124.51
32	a	408	PHO	CMC-C2C-C3C	2.13	128.95	124.94
31	b	617	CLA	CHD-C1D-ND	-2.13	122.50	124.45
31	g1	602	CLA	CHA-C1A-NA	-2.13	121.53	126.40
31	Y1	603	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
31	N1	602	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
47	s	606	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
31	B	603	CLA	CAC-C3C-C2C	-2.12	123.89	127.53
31	G	604	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
31	r	610	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
31	N1	614	CLA	CHA-C1A-NA	-2.12	121.53	126.40
47	Y	605	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
47	y	609	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
31	c	506	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
31	B	604	CLA	CHA-C1A-NA	-2.12	121.53	126.40
31	Y	608	CLA	CHA-C1A-NA	-2.12	121.53	126.40
31	R	609	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
49	N	622	XAT	C26-C27-C28	-2.12	121.50	125.99
31	C	504	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
46	h	101	RRX	C38-C26-C27	2.12	118.29	114.36
31	C	511	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
31	N	604	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
31	S	602	CLA	O2A-CGA-CBA	2.12	118.57	111.91
31	c1	501	CLA	CHA-C1A-NA	-2.12	121.54	126.40
31	c	502	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	C1	503	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	b	605	CLA	CHA-C1A-NA	-2.12	121.54	126.40
47	n1	601	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
47	g1	605	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
49	g	622	XAT	C18-C5-C6	-2.12	118.70	122.26
31	y	608	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
31	C	511	CLA	O1D-CGD-CBD	-2.12	120.14	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	603	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	g1	604	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
48	r	620	LUT	C31-C32-C33	-2.12	120.46	126.42
50	S1	623	NEX	C20-C13-C14	-2.12	119.95	122.92
31	S	611	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
47	G	601	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
31	c	507	CLA	CMA-C3A-C2A	2.12	122.38	113.83
31	Y1	603	CLA	C1D-ND-C4D	-2.12	104.83	106.33
41	D1	409	LHG	O7-C7-O9	-2.12	118.58	123.70
47	N	606	CHL	C1-C2-C3	-2.12	122.38	126.04
31	n	604	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
31	b1	606	CLA	CHA-C1A-NA	-2.12	121.54	126.40
31	C	507	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
47	s1	601	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
47	y1	605	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	G	602	CLA	C1-O2A-CGA	2.12	122.00	116.44
47	G1	607	CHL	C4D-CHA-C1A	2.12	123.83	121.25
31	b	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
47	N1	601	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	r	611	CLA	CHA-C1A-NA	-2.12	121.55	126.40
47	g	607	CHL	C4A-NA-C1A	2.12	107.66	106.71
31	C1	501	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	a1	407	CLA	C1D-ND-C4D	-2.12	104.83	106.33
33	C	515	BCR	C8-C7-C6	-2.12	121.26	127.20
47	N1	605	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	c	504	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	C1	510	CLA	CHA-C1A-NA	-2.12	121.55	126.40
33	B	619	BCR	C34-C9-C10	-2.12	119.96	122.92
33	c1	517	BCR	C19-C18-C17	2.12	122.19	118.94
47	N	605	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
47	S1	601	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
33	b1	618	BCR	C37-C22-C21	-2.12	119.96	122.92
31	R	613	CLA	C1D-ND-C4D	-2.12	104.83	106.33
31	n1	613	CLA	C1D-ND-C4D	-2.12	104.83	106.33
46	h1	101	RRX	C2-C1-C6	2.12	113.74	110.48
31	a	407	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
31	b1	608	CLA	C1-O2A-CGA	2.12	121.99	116.44
31	S1	613	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
50	R1	622	NEX	C5-C6-C1	2.12	121.80	119.70
47	g1	608	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	S	609	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	n	614	CLA	C1-O2A-CGA	2.11	121.99	116.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	606	CLA	CMA-C3A-C4A	2.11	117.46	111.77
31	Y	603	CLA	CHA-C1A-NA	-2.11	121.56	126.40
35	C1	521	LMG	O8-C28-O10	-2.11	118.26	123.59
47	N1	601	CHL	CHC-C1C-NC	2.11	127.41	124.20
31	N	614	CLA	CHA-C1A-NA	-2.11	121.56	126.40
31	g1	603	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
46	H1	101	RRX	C35-C13-C14	-2.11	119.96	122.92
48	g1	621	LUT	C19-C9-C10	-2.11	119.96	122.92
31	A1	407	CLA	C1D-ND-C4D	-2.11	104.83	106.33
31	G1	612	CLA	C1D-ND-C4D	-2.11	104.83	106.33
48	Y1	620	LUT	C39-C29-C28	2.11	121.41	118.08
31	n	604	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
56	r1	626	ERG	C12-C13-C17	-2.11	113.41	116.57
31	D	403	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
47	G	605	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
47	S1	607	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
47	g	609	CHL	CHC-C1C-NC	2.11	127.41	124.20
33	b	619	BCR	C28-C27-C26	-2.11	110.31	114.08
47	g1	607	CHL	C3C-C4C-NC	-2.11	108.20	110.57
31	C1	508	CLA	C1-O2A-CGA	2.11	121.99	116.44
31	n	613	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
31	g1	604	CLA	OBD-CAD-C3D	-2.11	123.44	128.52
31	a1	407	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
47	g1	609	CHL	CHC-C1C-NC	2.11	127.41	124.20
31	b	612	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	n1	614	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	R1	610	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
31	A	405	CLA	CAA-CBA-CGA	-2.11	107.08	113.25
31	g	610	CLA	CHA-C1A-NA	-2.11	121.56	126.40
46	h	101	RRX	C36-C18-C19	2.11	121.40	118.08
31	Y1	612	CLA	CMA-C3A-C4A	2.11	117.45	111.77
47	R	606	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	n	602	CLA	CHA-C1A-NA	-2.11	121.56	126.40
31	C	506	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	n1	612	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
31	r	603	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
31	R1	608	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
31	b1	606	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
47	S	607	CHL	C1B-CHB-C4A	-2.11	125.94	130.12
47	n	605	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	B1	617	CLA	CHA-C1A-NA	-2.11	121.56	126.40
48	G1	621	LUT	C19-C9-C10	-2.11	119.97	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	509	CLA	C1D-ND-C4D	-2.11	104.84	106.33
31	R1	602	CLA	C1D-ND-C4D	-2.11	104.84	106.33
31	y	602	CLA	CHA-C4D-ND	2.11	136.91	132.50
31	r	613	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
31	b1	605	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	s1	610	CLA	O2A-CGA-CBA	2.11	118.53	111.91
47	n	606	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	G1	602	CLA	C6-C5-C3	-2.11	107.92	113.45
50	N	623	NEX	C5-C4-C3	2.11	114.24	111.75
50	n	623	NEX	C5-C4-C3	2.11	114.24	111.75
31	N1	614	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
31	G1	604	CLA	O2A-CGA-CBA	2.11	118.53	111.91
31	B1	617	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
40	C	523	DGD	O1G-C1A-O1A	-2.11	118.27	123.59
31	N	614	CLA	C1D-ND-C4D	-2.11	104.84	106.33
47	g	606	CHL	C4A-NA-C1A	2.11	107.65	106.71
50	n1	623	NEX	C5-C4-C3	2.11	114.24	111.75
31	N	602	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	s	611	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
33	b	619	BCR	C23-C22-C21	2.11	122.18	118.94
47	s1	608	CHL	C1-O2A-CGA	2.11	121.97	116.44
48	r	620	LUT	C39-C29-C30	-2.11	119.97	122.92
47	g	609	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	c	501	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
37	b1	620	C7Z	C24-C25-C26	-2.11	116.15	120.85
35	b	622	LMG	O7-C10-O9	-2.11	118.61	123.70
31	r1	610	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
31	y1	603	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
48	N	620	LUT	C10-C11-C12	-2.11	116.64	123.22
48	y	620	LUT	C28-C29-C30	-2.11	115.71	118.94
31	s	610	CLA	CHA-C1A-NA	-2.11	121.57	126.40
50	G	623	NEX	O24-C25-C38	-2.11	112.53	115.06
31	b	613	CLA	C1-C2-C3	-2.11	122.40	126.04
31	n1	604	CLA	O2A-CGA-CBA	2.11	118.52	111.91
50	Y1	623	NEX	C5-C6-C1	2.11	121.79	119.70
31	g1	610	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
33	d1	404	BCR	C30-C25-C24	2.11	121.74	115.78
31	B	614	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	b1	602	CLA	O2A-CGA-CBA	2.11	118.52	111.91
35	A1	413	LMG	O7-C10-O9	-2.11	118.61	123.70
31	s	604	CLA	CAC-C3C-C4C	2.11	127.54	124.81
33	A1	411	BCR	C4-C5-C6	-2.11	119.67	122.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	613	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	y1	604	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	c	510	CLA	CMB-C2B-C3B	2.11	128.62	124.68
31	G	613	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	g	602	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	S1	604	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	G1	612	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
31	R	604	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
31	s1	610	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
31	S1	617	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
31	N1	614	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
31	G1	612	CLA	CHA-C1A-NA	-2.10	121.58	126.40
31	N1	613	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
31	R1	610	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
31	b	605	CLA	CMC-C2C-C3C	2.10	131.83	126.12
31	c1	513	CLA	CAA-C2A-C1A	2.10	118.87	111.97
31	D	403	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	y1	610	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
47	n	601	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
48	r1	620	LUT	C1-C6-C5	-2.10	119.65	122.61
41	n	624	LHG	O7-C7-O9	-2.10	118.62	123.70
31	A	410	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
31	s	604	CLA	CHA-C1A-NA	-2.10	121.58	126.40
40	c	519	DGD	O1G-C1A-O1A	-2.10	118.28	123.59
31	S	604	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	D	402	CLA	O2A-CGA-CBA	2.10	118.51	111.91
31	C	504	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
31	N	604	CLA	CHA-C1A-NA	-2.10	121.58	126.40
31	n1	603	CLA	CHA-C1A-NA	-2.10	121.58	126.40
49	Y	622	XAT	C20-C13-C14	-2.10	119.98	122.92
47	n	605	CHL	C1-C2-C3	-2.10	122.41	126.04
47	y1	609	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
31	B	614	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
31	b	615	CLA	CHA-C1A-NA	-2.10	121.58	126.40
31	r1	610	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
49	N1	622	XAT	C19-C9-C10	-2.10	119.98	122.92
31	B	602	CLA	CMA-C3A-C2A	2.10	122.31	113.83
49	r	622	XAT	C31-C32-C33	2.10	132.32	126.42
31	R1	612	CLA	C1D-ND-C4D	-2.10	104.84	106.33
48	n	620	LUT	C18-C5-C4	2.10	118.25	114.36
31	g	612	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
48	n1	620	LUT	C37-C21-C26	2.10	112.73	109.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	411	BCR	C38-C26-C25	-2.10	122.17	124.53
31	N	610	CLA	CBA-CAA-C2A	2.10	120.06	113.86
31	C	504	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
47	g	601	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
33	C1	514	BCR	C37-C22-C21	-2.10	119.98	122.92
31	C	507	CLA	C2A-C1A-CHA	2.10	127.53	123.86
31	C1	507	CLA	C2D-C1D-ND	2.10	111.65	110.10
31	Y	612	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
31	A1	405	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
47	Y1	605	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
33	c	516	BCR	C35-C13-C12	2.10	121.38	118.08
31	c	508	CLA	O2A-CGA-CBA	2.10	118.49	111.91
31	S1	609	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
33	c1	517	BCR	C8-C7-C6	-2.10	121.31	127.20
47	N1	607	CHL	C1B-CHB-C4A	-2.10	125.96	130.12
49	g1	622	XAT	C39-C29-C30	-2.10	119.98	122.92
31	s	612	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
31	a	405	CLA	CAC-C3C-C4C	2.10	127.53	124.81
31	c1	505	CLA	C2D-C1D-ND	2.10	111.65	110.10
31	n1	613	CLA	C2A-C1A-CHA	2.10	127.53	123.86
41	n	624	LHG	O8-C23-C24	2.10	118.49	111.91
31	S	612	CLA	C1D-ND-C4D	-2.10	104.84	106.33
47	n	605	CHL	CHC-C1C-NC	2.10	127.39	124.20
31	y1	614	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	C	502	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
31	R1	612	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
31	S	605	CLA	C2A-C1A-CHA	2.10	127.53	123.86
31	r1	608	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
31	r1	602	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
31	S1	610	CLA	CHA-C1A-NA	-2.10	121.60	126.40
31	n1	602	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
47	s	607	CHL	C4D-CHA-C1A	2.10	123.80	121.25
31	G1	604	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
31	B1	603	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
31	y1	608	CLA	C1D-ND-C4D	-2.10	104.85	106.33
47	Y1	606	CHL	CHB-C4A-NA	2.10	127.41	124.51
47	G	608	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
31	C	508	CLA	C6-C5-C3	-2.10	107.96	113.45
31	b1	615	CLA	OBD-CAD-C3D	-2.10	123.48	128.52
31	c	513	CLA	CHA-C1A-NA	-2.10	121.60	126.40
49	g	622	XAT	C19-C9-C10	-2.10	119.99	122.92
31	S	614	CLA	CMB-C2B-C3B	2.10	128.60	124.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	n	623	NEX	C11-C10-C9	2.10	130.30	127.31
47	Y	609	CHL	C4D-CHA-C1A	2.09	123.80	121.25
31	R	609	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
47	Y1	609	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
31	B1	610	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
31	c1	502	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
33	B1	618	BCR	C34-C9-C10	-2.09	119.99	122.92
50	n	623	NEX	C20-C13-C14	-2.09	119.99	122.92
31	N	603	CLA	CHA-C1A-NA	-2.09	121.60	126.40
47	g1	606	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
31	c	503	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
31	B	608	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
31	N	603	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
31	S1	603	CLA	O2A-CGA-CBA	2.09	118.48	111.91
31	R	602	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
31	a1	410	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
47	Y1	607	CHL	CHC-C1C-NC	2.09	127.38	124.20
31	B1	616	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
35	c1	521	LMG	O7-C10-O9	-2.09	118.64	123.70
50	N1	623	NEX	C4-C3-C2	2.09	114.81	110.77
31	b1	614	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
31	g	612	CLA	CHA-C1A-NA	-2.09	121.61	126.40
47	n1	605	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
31	b	612	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
31	a	406	CLA	O2A-CGA-CBA	2.09	118.47	111.91
31	Y1	608	CLA	O2A-CGA-CBA	2.09	118.47	111.91
37	b1	620	C7Z	C21-C26-C27	2.09	121.70	115.78
31	N1	603	CLA	C1D-ND-C4D	-2.09	104.85	106.33
31	y1	610	CLA	C1D-ND-C4D	-2.09	104.85	106.33
31	b1	610	CLA	CHA-C1A-NA	-2.09	121.61	126.40
49	G1	622	XAT	C20-C13-C14	-2.09	119.99	122.92
53	y	625	SPH	C1-C2-C3	-2.09	108.53	113.03
31	Y	608	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
31	S1	603	CLA	C2A-C1A-CHA	2.09	127.51	123.86
48	S1	621	LUT	C31-C32-C33	-2.09	120.54	126.42
49	n1	622	XAT	C19-C9-C10	-2.09	120.00	122.92
31	s	612	CLA	CHA-C1A-NA	-2.09	121.61	126.40
48	N	620	LUT	C39-C29-C28	2.09	121.37	118.08
31	C1	502	CLA	O2A-CGA-CBA	2.09	118.47	111.91
31	S1	612	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	C1	506	CLA	CHA-C1A-NA	-2.09	121.61	126.40
31	s1	613	CLA	CHA-C1A-NA	-2.09	121.61	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D1	403	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
31	g1	604	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	s	602	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	C	508	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
31	b	610	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
47	N	601	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
31	s1	602	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	C1	508	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
31	S1	603	CLA	C1-O2A-CGA	2.09	121.92	116.44
31	y1	602	CLA	CHA-C1A-NA	-2.09	121.62	126.40
33	c	514	BCR	C23-C24-C25	-2.09	121.34	127.20
47	y	609	CHL	C1-C2-C3	-2.09	122.43	126.04
31	C1	511	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
31	c	503	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c1	503	CLA	CHA-C1A-NA	-2.09	121.62	126.40
31	C	508	CLA	O2A-CGA-CBA	2.09	118.46	111.91
31	S1	602	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
31	c	507	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
48	r1	620	LUT	C31-C32-C33	-2.09	120.56	126.42
31	B1	614	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
31	g1	612	CLA	C1D-ND-C4D	-2.09	104.85	106.33
47	G1	601	CHL	CHC-C1C-NC	2.09	127.37	124.20
33	c	515	BCR	C3-C4-C5	-2.09	110.35	114.08
31	s1	602	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
33	D1	404	BCR	C38-C26-C27	2.09	117.62	113.62
31	g1	613	CLA	CMB-C2B-C3B	2.09	128.58	124.68
31	b	608	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	C1	512	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
31	y	604	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
50	r	623	NEX	C40-C33-C34	-2.09	120.00	122.92
31	c1	503	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	G	611	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
40	c1	519	DGD	C2G-O2G-C1B	-2.08	112.66	117.79
31	c	503	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
47	Y1	609	CHL	C4A-NA-C1A	2.08	107.64	106.71
31	y	610	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	g1	613	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	R	613	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
45	f	101	HEM	CBD-CAD-C3D	-2.08	106.84	112.63
31	S1	610	CLA	C1-O2A-CGA	2.08	121.91	116.44
31	D1	403	CLA	CHA-C1A-NA	-2.08	121.63	126.40
31	c1	513	CLA	CMD-C2D-C3D	-2.08	122.82	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S1	602	CLA	CHA-C1A-NA	-2.08	121.63	126.40
31	g1	610	CLA	C6-C5-C3	-2.08	108.00	113.45
31	Y1	602	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
35	D	411	LMG	C8-O7-C10	-2.08	112.67	117.79
50	g	623	NEX	O24-C25-C24	-2.08	111.82	113.38
31	B1	603	CLA	CHA-C1A-NA	-2.08	121.63	126.40
31	c1	501	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
31	y1	602	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
47	s1	606	CHL	CHD-C4C-C3C	2.08	127.90	124.84
31	c1	505	CLA	OBD-CAD-C3D	-2.08	123.51	128.52
47	G1	605	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
31	c	507	CLA	CMA-C3A-C4A	2.08	117.37	111.77
31	C	505	CLA	C1D-ND-C4D	-2.08	104.86	106.33
31	R1	610	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
31	r1	602	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	s1	605	CLA	C2A-C1A-CHA	2.08	127.50	123.86
31	s	603	CLA	O2A-CGA-CBA	2.08	118.43	111.91
33	C	517	BCR	C34-C9-C10	-2.08	120.01	122.92
47	y	606	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
31	c1	503	CLA	CMA-C3A-C4A	2.08	117.36	111.77
31	c1	512	CLA	C2A-C1A-CHA	2.08	127.50	123.86
31	C	502	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	N1	614	CLA	C1-O2A-CGA	2.08	121.90	116.44
31	Y	610	CLA	CMA-C3A-C4A	2.08	117.36	111.77
31	r1	602	CLA	CMC-C2C-C1C	2.08	128.21	125.04
31	y	611	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
31	b	605	CLA	O2A-CGA-CBA	2.08	118.43	111.91
31	g	602	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
31	r	604	CLA	O2A-CGA-CBA	2.08	118.43	111.91
31	B1	608	CLA	C1-O2A-CGA	2.08	121.90	116.44
31	s	602	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
31	Y1	604	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
31	g1	614	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
31	C	511	CLA	C1D-ND-C4D	-2.08	104.86	106.33
31	c1	513	CLA	C2A-C1A-CHA	2.08	127.49	123.86
47	y	601	CHL	C4A-NA-C1A	2.08	107.64	106.71
49	R1	621	XAT	C24-C23-C22	-2.08	106.76	110.77
31	a	407	CLA	O2A-CGA-CBA	2.08	118.43	111.91
31	s	609	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
31	g1	610	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
31	G	613	CLA	C1-O2A-CGA	2.08	121.89	116.44
48	S	620	LUT	C10-C11-C12	-2.08	116.74	123.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	603	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
31	c1	511	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
31	y1	604	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
31	B1	613	CLA	O2A-CGA-CBA	2.08	118.42	111.91
31	a1	410	CLA	CHA-C1A-NA	-2.08	121.64	126.40
41	c	625	LHG	O8-C23-O10	-2.08	118.35	123.59
31	n	610	CLA	CHA-C4D-ND	2.08	136.84	132.50
31	g	602	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
44	D1	405	PL9	C37-C38-C39	-2.08	122.66	127.66
33	c1	516	BCR	C35-C13-C12	2.08	121.35	118.08
48	N	620	LUT	C20-C13-C12	2.08	121.35	118.08
50	g	623	NEX	C31-C32-C33	2.08	132.25	126.42
46	H	101	RRX	C36-C18-C17	-2.08	120.02	122.92
31	r1	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	c1	504	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
31	n	613	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
33	a	411	BCR	C19-C18-C17	2.08	122.13	118.94
47	G1	601	CHL	CHA-C1A-NA	-2.08	121.64	126.40
31	r	609	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
31	S1	611	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
31	C	512	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
31	G	610	CLA	CHA-C1A-NA	-2.07	121.65	126.40
31	y1	613	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	g1	611	CLA	O2A-CGA-CBA	2.07	118.42	111.91
31	b1	611	CLA	CMA-C3A-C4A	2.07	117.35	111.77
31	C1	508	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	n	610	CLA	CMB-C2B-C3B	2.07	128.56	124.68
35	C	521	LMG	O7-C10-O9	-2.07	118.69	123.70
31	r1	612	CLA	O2A-CGA-CBA	2.07	118.42	111.91
31	C1	509	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
33	B1	619	BCR	C34-C9-C10	-2.07	120.02	122.92
49	Y	622	XAT	C19-C9-C10	-2.07	120.02	122.92
47	y	605	CHL	CHD-C4C-C3C	2.07	127.89	124.84
31	G1	614	CLA	C1D-ND-C4D	-2.07	104.86	106.33
48	n1	621	LUT	C20-C13-C12	2.07	121.34	118.08
31	n	611	CLA	O2A-CGA-CBA	2.07	118.41	111.91
47	g1	607	CHL	C4D-CHA-C1A	2.07	123.77	121.25
31	R	611	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	b	616	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
47	n	601	CHL	CHD-C4C-C3C	2.07	127.89	124.84
31	N	611	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
31	G	613	CLA	CAA-C2A-C3A	-2.07	107.10	112.78

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n1	602	CLA	CMA-C3A-C4A	2.07	117.34	111.77
31	G	611	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	c	504	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
48	n1	621	LUT	C18-C5-C4	2.07	118.19	114.36
31	g1	604	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	A1	405	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	s1	603	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
33	C1	517	BCR	C31-C1-C6	-2.07	106.94	110.30
49	r1	621	XAT	O4-C5-C4	-2.07	111.83	113.38
31	r1	612	CLA	CMA-C3A-C4A	2.07	117.34	111.77
33	D	404	BCR	C30-C25-C26	-2.07	119.70	122.61
47	S1	608	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
45	f	101	HEM	CAD-CBD-CGD	-2.07	109.15	113.60
31	g1	602	CLA	CAC-C3C-C4C	2.07	127.50	124.81
31	S	604	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	S1	609	CLA	C1-C2-C3	-2.07	122.46	126.04
31	r	602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	C1	501	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	b1	607	CLA	CHA-C1A-NA	-2.07	121.66	126.40
31	y1	613	CLA	CHA-C1A-NA	-2.07	121.66	126.40
43	d	401	BCT	O3-C-O1	-2.07	114.18	119.55
47	n	606	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
31	B1	610	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
31	B1	605	CLA	C2A-C1A-CHA	2.07	127.48	123.86
31	a	405	CLA	CMC-C2C-C1C	2.07	128.19	125.04
47	g	601	CHL	C1-C2-C3	-2.07	122.47	126.04
31	r1	604	CLA	CHA-C1A-NA	-2.07	121.66	126.40
31	s	604	CLA	C1D-ND-C4D	-2.07	104.87	106.33
31	Y1	613	CLA	C1D-ND-C4D	-2.07	104.87	106.33
48	g	620	LUT	C31-C32-C33	-2.07	120.61	126.42
48	N	620	LUT	C15-C35-C34	-2.07	119.24	123.47
31	B	614	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	R	612	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	Y	603	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	Y	610	CLA	CHA-C1A-NA	-2.07	121.66	126.40
31	d	402	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
31	c	513	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
47	S	608	CHL	CHB-C4A-NA	2.07	127.37	124.51
31	g	604	CLA	CHA-C1A-NA	-2.07	121.67	126.40
31	N	603	CLA	O2A-CGA-CBA	2.07	118.39	111.91
48	G	621	LUT	C8-C7-C6	-2.07	121.40	127.20
47	y	605	CHL	CHC-C1C-NC	2.07	127.34	124.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	D1	405	PL9	C27-C28-C29	-2.07	122.69	127.66
44	D	405	PL9	C50-C49-C48	-2.07	116.68	122.65
31	S1	611	CLA	C2A-C1A-CHA	2.07	127.47	123.86
31	c1	502	CLA	C1D-ND-C4D	-2.07	104.87	106.33
31	s1	609	CLA	C1-O2A-CGA	2.07	121.86	116.44
47	R	606	CHL	C2C-C3C-C4C	2.06	107.96	106.49
47	y1	606	CHL	CHC-C1C-NC	2.06	127.33	124.20
47	N	601	CHL	C1B-CHB-C4A	-2.06	126.03	130.12
31	d	402	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
47	g	601	CHL	CHD-C4C-C3C	2.06	127.87	124.84
31	b	602	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
31	n1	604	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	n	610	CLA	CBA-CAA-C2A	2.06	119.95	113.86
31	C1	508	CLA	C1C-C2C-C3C	-2.06	104.79	106.96
31	n	611	CLA	C1-O2A-CGA	2.06	121.86	116.44
37	b	620	C7Z	C40-C33-C34	-2.06	120.03	122.92
49	R1	621	XAT	C40-C33-C34	-2.06	120.03	122.92
47	G	609	CHL	C1-C2-C3	-2.06	122.47	126.04
31	B1	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	g1	604	CLA	CMB-C2B-C3B	2.06	128.54	124.68
31	C	504	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	N1	614	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	b	608	CLA	CMB-C2B-C3B	2.06	128.54	124.68
31	B1	617	CLA	C1-O2A-CGA	2.06	121.85	116.44
31	N	604	CLA	CMA-C3A-C4A	2.06	117.31	111.77
31	n	612	CLA	CMA-C3A-C4A	2.06	117.31	111.77
31	Y1	604	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
50	g	623	NEX	C20-C13-C14	-2.06	120.03	122.92
31	A	405	CLA	C6-C7-C8	-2.06	109.25	115.92
31	b1	607	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
34	B1	621	SQD	O8-S-C6	-2.06	102.45	105.74
33	C1	517	BCR	C33-C5-C4	2.06	117.58	113.62
31	y1	614	CLA	C2D-C1D-ND	2.06	111.62	110.10
33	b	619	BCR	C1-C6-C5	-2.06	119.71	122.61
40	c1	518	DGD	O6D-C5D-C6D	2.06	110.83	106.67
31	y	603	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
49	r	622	XAT	C12-C13-C14	2.06	122.10	118.94
31	D	402	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
31	S	613	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
48	S	621	LUT	C1-C6-C7	2.06	121.61	115.78
31	A	405	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
48	S1	620	LUT	C20-C13-C12	2.06	121.32	118.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	406	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	A1	410	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	R	604	CLA	C1-O2A-CGA	2.06	121.85	116.44
31	C1	509	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	c	510	CLA	C11-C10-C8	-2.06	109.26	115.92
31	d	402	CLA	CHA-C1A-NA	-2.06	121.68	126.40
53	a1	414	SPH	C3-C4-C5	-2.06	120.20	124.79
47	g1	606	CHL	CHD-C4C-C3C	2.06	127.87	124.84
31	a1	405	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	b	608	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	C	502	CLA	O2A-CGA-CBA	2.06	118.36	111.91
31	g	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	d1	402	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	r1	612	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
47	R	607	CHL	C4A-NA-C1A	2.06	107.63	106.71
31	c	512	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
31	r	602	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
33	c1	514	BCR	C29-C28-C27	2.06	115.97	111.38
31	c	503	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	B	613	CLA	CHA-C1A-NA	-2.06	121.69	126.40
31	G	603	CLA	CHA-C1A-NA	-2.06	121.69	126.40
50	G1	623	NEX	C20-C13-C14	-2.06	120.04	122.92
31	s	610	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
31	G1	611	CLA	CAC-C3C-C4C	2.06	127.48	124.81
31	B1	616	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
31	Y1	602	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
31	c	502	CLA	CHA-C1A-NA	-2.06	121.69	126.40
40	B1	623	DGD	O2G-C1B-O1B	-2.06	118.73	123.70
50	r1	622	NEX	C20-C13-C14	-2.06	120.04	122.92
31	s1	602	CLA	CHA-C1A-NA	-2.05	121.69	126.40
31	G1	602	CLA	CAC-C3C-C4C	2.05	127.48	124.81
31	S	611	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
31	b1	602	CLA	C2A-C1A-CHA	2.05	127.45	123.86
31	C1	504	CLA	O2A-CGA-CBA	2.05	118.35	111.91
31	n	614	CLA	CMB-C2B-C3B	2.05	128.52	124.68
31	s	614	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
31	c	509	CLA	CMA-C3A-C4A	2.05	117.29	111.77
31	B1	607	CLA	C2D-C1D-ND	2.05	111.62	110.10
31	n1	603	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
31	S	610	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
31	G1	611	CLA	O2A-CGA-CBA	2.05	118.35	111.91
31	R1	610	CLA	CHA-C1A-NA	-2.05	121.70	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	509	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	n	604	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	c1	501	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	n1	602	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
47	g1	606	CHL	C1B-CHB-C4A	-2.05	126.05	130.12
55	R1	625	LMT	C1'-O5'-C5'	-2.05	109.66	113.69
31	n1	603	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	n1	604	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	C1	506	CLA	C1D-ND-C4D	-2.05	104.88	106.33
31	a1	410	CLA	C1D-ND-C4D	-2.05	104.88	106.33
37	B1	620	C7Z	C8-C7-C6	-2.05	121.44	127.20
31	S	617	CLA	CMB-C2B-C3B	2.05	128.51	124.68
31	c1	506	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
35	a	413	LMG	O7-C10-O9	-2.05	118.75	123.70
31	g	612	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	g1	610	CLA	CMB-C2B-C3B	2.05	128.51	124.68
47	R	606	CHL	C1B-CHB-C4A	-2.05	126.06	130.12
31	S1	604	CLA	C1-O2A-CGA	2.05	121.82	116.44
31	a	405	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	C1	502	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	r1	604	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	S1	610	CLA	CMB-C2B-C3B	2.05	128.51	124.68
48	S	620	LUT	C36-C21-C26	2.05	112.65	109.55
33	C1	515	BCR	C4-C5-C6	-2.05	119.76	122.73
47	r1	606	CHL	C3C-C4C-NC	-2.05	108.27	110.57
31	n	612	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
33	C	516	BCR	C35-C13-C12	2.05	121.31	118.08
48	R1	620	LUT	C1-C6-C5	-2.05	119.73	122.61
31	y1	611	CLA	O2A-CGA-CBA	2.05	118.34	111.91
31	r	611	CLA	C1D-ND-C4D	-2.05	104.88	106.33
31	N	614	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	S	613	CLA	C2A-C1A-CHA	2.05	127.44	123.86
31	C1	513	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
31	Y	614	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
48	G	621	LUT	C31-C32-C33	-2.05	120.66	126.42
48	Y	620	LUT	C11-C10-C9	-2.05	124.39	127.31
33	c	517	BCR	C37-C22-C21	-2.05	120.06	122.92
31	D1	402	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
31	S	612	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	r1	602	CLA	CHA-C1A-NA	-2.05	121.71	126.40
33	C1	514	BCR	C31-C1-C6	-2.05	106.98	110.30
47	N	607	CHL	CHA-C1A-NA	-2.05	121.71	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	n1	622	XAT	C26-C27-C28	-2.05	121.67	125.99
31	R	613	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
47	y1	607	CHL	CHA-C1A-NA	-2.05	121.71	126.40
48	Y1	620	LUT	C20-C13-C12	2.05	121.30	118.08
31	R1	602	CLA	CAC-C3C-C4C	2.05	127.46	124.81
31	B1	607	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
31	B1	614	CLA	OBD-CAD-C3D	-2.05	123.60	128.52
31	N1	604	CLA	CMA-C3A-C4A	2.05	117.27	111.77
47	n1	606	CHL	C4D-CHA-C1A	2.05	123.74	121.25
31	y	608	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	G	604	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
31	c	508	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
31	D	402	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
47	Y1	605	CHL	C1B-CHB-C4A	-2.04	126.07	130.12
31	G1	610	CLA	CMB-C2B-C3B	2.04	128.50	124.68
31	B	609	CLA	O2A-CGA-CBA	2.04	118.32	111.91
31	g	603	CLA	O2A-CGA-CBA	2.04	118.32	111.91
47	S	606	CHL	C4A-NA-C1A	2.04	107.62	106.71
47	S1	607	CHL	C4A-NA-C1A	2.04	107.62	106.71
31	b	605	CLA	C2A-C1A-CHA	2.04	127.43	123.86
55	r1	625	LMT	C3B-C4B-C5B	-2.04	106.59	110.24
41	d1	408	LHG	C5-O7-C7	-2.04	112.76	117.79
31	y1	608	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
31	d1	402	CLA	C4-C3-C5	2.04	118.71	115.27
44	D	405	PL9	C37-C38-C39	-2.04	122.74	127.66
31	b	615	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
33	C	516	BCR	C38-C26-C27	2.04	117.54	113.62
31	C1	513	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
31	B	616	CLA	C1D-ND-C4D	-2.04	104.88	106.33
31	y	613	CLA	C1D-ND-C4D	-2.04	104.88	106.33
37	b	620	C7Z	C20-C13-C14	-2.04	120.06	122.92
47	N1	608	CHL	CHD-C4C-C3C	2.04	127.84	124.84
31	s	605	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
48	s	620	LUT	C31-C32-C33	-2.04	120.68	126.42
32	a1	408	PHO	C1-C2-C3	-2.04	122.51	126.04
48	s	620	LUT	C36-C21-C26	2.04	112.64	109.55
31	B1	606	CLA	CMA-C3A-C4A	2.04	117.26	111.77
31	C	504	CLA	O2A-CGA-CBA	2.04	118.31	111.91
31	r	610	CLA	C2A-C1A-CHA	2.04	127.43	123.86
31	R1	604	CLA	C2D-C1D-ND	2.04	111.61	110.10
31	C1	509	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
31	Y	610	CLA	OBD-CAD-C3D	-2.04	123.61	128.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A1	405	CLA	CMC-C2C-C1C	-2.04	121.93	125.04
31	A1	405	CLA	C3C-C4C-NC	2.04	112.86	110.57
31	b1	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
47	G1	606	CHL	CHA-C1A-NA	-2.04	121.73	126.40
31	B	617	CLA	C1-O2A-CGA	2.04	121.80	116.44
31	r1	604	CLA	C1D-ND-C4D	-2.04	104.89	106.33
33	b1	619	BCR	C37-C22-C21	-2.04	120.07	122.92
31	c1	502	CLA	CMC-C2C-C3C	2.04	131.65	126.12
31	n1	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	g1	603	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
33	C	517	BCR	C2-C3-C4	-2.04	106.82	111.38
31	s	603	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
31	Y1	603	CLA	C1-O2A-CGA	2.04	121.79	116.44
31	Y	613	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
31	r1	602	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
47	g	608	CHL	C3A-C2A-C1A	2.04	104.39	101.34
31	R	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	S1	614	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
31	N1	603	CLA	C1-O2A-CGA	2.04	121.79	116.44
31	D	403	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
31	G	614	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
47	n1	608	CHL	C4D-CHA-C1A	2.04	123.73	121.25
31	R1	608	CLA	O2A-CGA-CBA	2.04	118.30	111.91
31	c	512	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	b1	605	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
31	S1	604	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
31	y1	614	CLA	O2A-CGA-CBA	2.04	118.30	111.91
31	a	410	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
31	N1	613	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
31	G	612	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
47	S	601	CHL	C1B-CHB-C4A	-2.04	126.08	130.12
47	g1	605	CHL	CHD-C4C-C3C	2.04	127.83	124.84
31	b	606	CLA	CAC-C3C-C4C	2.04	127.45	124.81
31	s1	603	CLA	C2A-C1A-CHA	2.04	127.42	123.86
31	S	602	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
31	A	410	CLA	CHA-C1A-NA	-2.04	121.74	126.40
31	s1	602	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
31	c1	504	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	B	605	CLA	CMA-C3A-C2A	2.03	122.03	113.83
50	y1	623	NEX	C4-C3-C2	2.03	114.70	110.77
33	B	618	BCR	C38-C26-C25	-2.03	122.24	124.53
31	b	611	CLA	O1D-CGD-CBD	-2.03	120.32	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	609	CLA	O2A-CGA-CBA	2.03	118.29	111.91
31	y1	603	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	g1	602	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
44	d	405	PL9	O2-C1-C2	-2.03	117.12	121.78
31	G1	614	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	Y1	604	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	S	617	CLA	C1-O2A-CGA	2.03	121.78	116.44
31	B	615	CLA	C2A-C1A-CHA	2.03	127.41	123.86
49	R1	621	XAT	C19-C9-C10	-2.03	120.08	122.92
49	y1	622	XAT	C20-C13-C14	-2.03	120.08	122.92
31	b	603	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
31	g	614	CLA	C1D-ND-C4D	-2.03	104.89	106.33
31	R1	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	c	511	CLA	CHA-C1A-NA	-2.03	121.75	126.40
47	Y1	609	CHL	CHC-C1C-NC	2.03	127.28	124.20
31	c	511	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
47	G	608	CHL	CHD-C4C-C3C	2.03	127.82	124.84
47	g	606	CHL	CHD-C4C-C3C	2.03	127.82	124.84
31	N	602	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
31	c	506	CLA	CMB-C2B-C3B	2.03	128.48	124.68
31	G1	603	CLA	C1D-ND-C4D	-2.03	104.89	106.33
50	y1	623	NEX	C11-C12-C13	2.03	132.12	126.42
31	S1	602	CLA	CMC-C2C-C1C	2.03	128.13	125.04
31	y1	614	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
31	S1	612	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
31	Y	613	CLA	C1-O2A-CGA	2.03	121.77	116.44
31	n1	604	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
31	B	616	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
31	n	614	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
33	a	411	BCR	C4-C5-C6	-2.03	119.78	122.73
31	A1	407	CLA	C2A-C1A-CHA	2.03	127.41	123.86
41	D1	409	LHG	O8-C23-O10	-2.03	118.47	123.59
31	B1	608	CLA	CAC-C3C-C4C	2.03	127.44	124.81
47	r	606	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
31	g	604	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	N1	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
31	b	614	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	g1	604	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
33	c1	517	BCR	C29-C30-C25	2.03	113.60	110.48
31	b1	606	CLA	C1D-ND-C4D	-2.03	104.89	106.33
31	G	602	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	s1	614	CLA	CHA-C1A-NA	-2.03	121.76	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s1	609	CLA	C2A-C1A-CHA	2.03	127.40	123.86
47	r1	607	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
47	N	607	CHL	C4D-CHA-C1A	2.03	123.72	121.25
47	Y	606	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
31	B1	613	CLA	CMC-C2C-C1C	2.03	128.12	125.04
35	J	101	LMG	C8-O7-C10	-2.03	112.80	117.79
31	D	403	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	b1	608	CLA	CHA-C1A-NA	-2.03	121.76	126.40
50	r	623	NEX	C19-C9-C10	-2.03	120.09	122.92
31	S1	609	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
31	Y	613	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	S1	613	CLA	CHA-C1A-NA	-2.02	121.76	126.40
50	G	623	NEX	C16-C1-C6	-2.02	108.66	110.47
31	b1	612	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	b1	607	CLA	CMB-C2B-C3B	2.02	128.47	124.68
31	n1	603	CLA	O2A-CGA-CBA	2.02	118.26	111.91
31	b1	616	CLA	C1-O2A-CGA	2.02	121.75	116.44
31	n	604	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	r1	610	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
31	b	609	CLA	C2A-C1A-CHA	2.02	127.40	123.86
44	d	405	PL9	C42-C43-C44	-2.02	122.79	127.66
31	b1	603	CLA	CMB-C2B-C3B	2.02	128.46	124.68
31	B	603	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	Y1	612	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
33	c	515	BCR	C15-C14-C13	-2.02	124.42	127.31
47	N	601	CHL	CHD-C4C-C3C	2.02	127.81	124.84
47	N1	608	CHL	C4A-NA-C1A	2.02	107.61	106.71
31	b1	612	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
31	R	610	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
31	S	617	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	Y1	604	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
31	s1	613	CLA	C1-O2A-CGA	2.02	121.75	116.44
48	s1	621	LUT	C40-C33-C34	-2.02	120.09	122.92
31	r1	609	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
31	N	614	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
31	A	410	CLA	CMB-C2B-C3B	2.02	128.46	124.68
31	A1	406	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
31	s1	617	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
31	b	616	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
40	b1	623	DGD	O1G-C1A-O1A	-2.02	118.49	123.59
31	B1	610	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	A	407	CLA	O2D-CGD-O1D	-2.02	119.89	123.84

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	G1	601	CHL	C4A-NA-C1A	2.02	107.61	106.71
33	c1	514	BCR	C1-C6-C5	-2.02	119.77	122.61
31	n	604	CLA	C2A-C1A-CHA	2.02	127.39	123.86
31	r	609	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
31	s1	611	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
47	y	607	CHL	CMA-C3A-C2A	2.02	121.97	113.83
33	B1	618	BCR	C40-C30-C25	-2.02	107.02	110.30
47	n	606	CHL	C3A-C2A-C1A	2.02	104.36	101.34
31	C1	513	CLA	CHA-C1A-NA	-2.02	121.78	126.40
31	N	602	CLA	CMC-C2C-C1C	2.02	128.11	125.04
33	b	618	BCR	C35-C13-C12	2.02	121.26	118.08
33	A1	411	BCR	C35-C13-C12	2.02	121.26	118.08
31	y	613	CLA	CHA-C1A-NA	-2.02	121.78	126.40
31	R	602	CLA	C1-O2A-CGA	2.02	121.74	116.44
48	s1	620	LUT	C19-C9-C10	-2.02	120.10	122.92
31	c1	513	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
31	b	604	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
31	G	603	CLA	CMC-C2C-C1C	2.02	128.11	125.04
47	G	605	CHL	CHD-C4C-C3C	2.02	127.81	124.84
31	B	607	CLA	CAC-C3C-C4C	2.02	127.43	124.81
43	D1	401	BCT	O3-C-O1	-2.02	114.31	119.55
47	y	606	CHL	CHA-C1A-NA	-2.02	121.78	126.40
31	B1	617	CLA	C1D-ND-C4D	-2.02	104.90	106.33
47	G	607	CHL	CHD-C4C-C3C	2.02	127.81	124.84
47	N1	606	CHL	CHD-C4C-C3C	2.02	127.81	124.84
48	Y	621	LUT	C3-C4-C5	-2.02	107.84	111.85
33	D	404	BCR	C35-C13-C12	2.02	121.25	118.08
33	c	515	BCR	C37-C22-C23	2.02	121.25	118.08
31	r	613	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	S1	605	CLA	C2A-C1A-CHA	2.02	127.39	123.86
47	g1	606	CHL	CHA-C1A-NA	-2.02	121.78	126.40
34	c1	526	SQD	O8-S-C6	-2.02	102.53	105.74
31	b1	617	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
31	A1	405	CLA	C1-O2A-CGA	2.02	121.73	116.44
47	g	607	CHL	CHD-C4C-C3C	2.02	127.80	124.84
47	n1	605	CHL	CHD-C4C-C3C	2.02	127.80	124.84
31	b	616	CLA	CMB-C2B-C3B	2.02	128.45	124.68
47	n	601	CHL	C1B-CHB-C4A	-2.02	126.12	130.12
31	g1	602	CLA	CMD-C2D-C3D	-2.02	122.98	127.61
47	s	601	CHL	C4A-NA-C1A	2.02	107.61	106.71
41	D1	408	LHG	O7-C7-O9	-2.02	118.83	123.70
31	R1	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b1	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
47	g	605	CHL	C1-O2A-CGA	2.01	122.58	116.73
31	s	605	CLA	C2A-C1A-CHA	2.01	127.38	123.86
31	c1	509	CLA	CHA-C1A-NA	-2.01	121.78	126.40
31	a	407	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
31	n1	614	CLA	CMB-C2B-C3B	2.01	128.45	124.68
47	s	607	CHL	CHD-C4C-C3C	2.01	127.80	124.84
31	C	513	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
47	n1	609	CHL	CHC-C1C-NC	2.01	127.26	124.20
31	B	607	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
31	c	505	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
47	n	609	CHL	C1-O2A-CGA	2.01	121.73	116.44
31	y	602	CLA	CMB-C2B-C3B	2.01	128.45	124.68
31	s1	604	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
31	S1	610	CLA	CAC-C3C-C4C	2.01	127.42	124.81
48	G	621	LUT	C16-C1-C6	-2.01	107.03	110.30
31	a1	406	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
32	A1	408	PHO	O2A-CGA-O1A	-2.01	118.51	123.59
40	C	519	DGD	O1G-C1A-O1A	-2.01	118.51	123.59
46	h1	101	RRX	C36-C18-C17	-2.01	120.10	122.92
31	g1	613	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
33	d	404	BCR	C15-C14-C13	2.01	130.18	127.31
31	b	616	CLA	CAC-C3C-C4C	2.01	127.42	124.81
47	g	605	CHL	CHC-C1C-NC	2.01	127.26	124.20
31	g	614	CLA	CMB-C2B-C3B	2.01	128.44	124.68
31	C	508	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
31	y	602	CLA	C2C-C1C-NC	2.01	111.86	109.97
31	G1	604	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
31	S1	605	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
48	r1	620	LUT	C22-C23-C24	-2.01	109.45	111.74
46	H	101	RRX	C34-C9-C10	-2.01	120.11	122.92
48	s1	621	LUT	C1-C6-C7	2.01	121.47	115.78
31	B1	609	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
44	d1	405	PL9	O1-C4-C3	-2.01	118.50	120.72
31	a1	406	CLA	C6-C5-C3	-2.01	108.18	113.45
31	b	615	CLA	CAC-C3C-C2C	-2.01	124.09	127.53
31	c1	508	CLA	O2A-CGA-CBA	2.01	118.22	111.91
46	H	101	RRX	C8-C7-C6	-2.01	121.55	127.20
33	b	618	BCR	C37-C22-C21	-2.01	120.11	122.92
31	b	603	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
31	y	603	CLA	CHA-C1A-NA	-2.01	121.79	126.40
31	g1	613	CLA	O2D-CGD-O1D	-2.01	119.91	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y1	613	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
45	f	101	HEM	CBA-CAA-C2A	-2.01	109.19	112.62
33	c	516	BCR	C1-C6-C7	2.01	121.46	115.78
47	G	607	CHL	CHA-C1A-NA	-2.01	121.80	126.40
31	S1	604	CLA	CMB-C2B-C3B	2.01	128.44	124.68
31	G1	610	CLA	C1C-C2C-C3C	-2.01	104.84	106.96
31	B1	611	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
31	n1	610	CLA	C1D-ND-C4D	-2.01	104.91	106.33
31	S1	612	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
48	G	620	LUT	C19-C9-C10	-2.01	120.11	122.92
31	r	602	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
31	B	616	CLA	CMA-C3A-C2A	2.01	121.93	113.83
31	B	615	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	b1	604	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
31	C1	510	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
31	s1	611	CLA	C1D-ND-C4D	-2.01	104.91	106.33
31	n	603	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	c1	503	CLA	CMA-C3A-C2A	2.01	121.92	113.83
31	R	610	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	y1	602	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
47	g1	609	CHL	CHD-C4C-C3C	2.01	127.79	124.84
31	r1	612	CLA	CAC-C3C-C4C	2.01	127.41	124.81
40	c1	519	DGD	O2G-C1B-O1B	-2.01	118.85	123.70
33	A1	411	BCR	C34-C9-C10	-2.01	120.11	122.92
33	d1	404	BCR	C8-C9-C10	2.01	122.02	118.94
33	a	411	BCR	C38-C26-C27	2.01	117.47	113.62
31	y1	611	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
31	N	610	CLA	CAC-C3C-C4C	2.01	127.41	124.81
31	B	617	CLA	C1C-C2C-C3C	-2.00	104.85	106.96
31	g	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	B1	607	CLA	C2A-C1A-CHA	2.00	127.36	123.86
31	B1	612	CLA	CHA-C1A-NA	-2.00	121.81	126.40
33	a1	411	BCR	C38-C26-C27	2.00	117.47	113.62
50	y	623	NEX	C5-C4-C3	2.00	114.12	111.75
47	G	606	CHL	CHD-C4C-C3C	2.00	127.78	124.84
31	r	609	CLA	C1D-ND-C4D	-2.00	104.91	106.33
31	Y1	604	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	b1	615	CLA	C2D-C1D-ND	2.00	111.58	110.10
47	n1	608	CHL	C1B-CHB-C4A	-2.00	126.15	130.12
31	y	610	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
47	s	608	CHL	CHC-C1C-NC	2.00	127.24	124.20
34	A1	412	SQD	O8-S-C6	-2.00	102.55	105.74

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R1	602	CLA	C1C-C2C-C3C	-2.00	104.85	106.96
31	B1	605	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
31	R	602	CLA	C1D-ND-C4D	-2.00	104.91	106.33
31	C1	511	CLA	C1D-ND-C4D	-2.00	104.91	106.33
31	S	610	CLA	CMC-C2C-C1C	2.00	128.09	125.04
31	s1	611	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
31	G	612	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
48	n1	621	LUT	C10-C11-C12	-2.00	116.97	123.22
31	A	406	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	n	613	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
31	G	614	CLA	CHA-C1A-NA	-2.00	121.82	126.40
31	r	609	CLA	C1-O2A-CGA	2.00	121.69	116.44
50	N	623	NEX	C40-C33-C32	2.00	121.23	118.08
49	G1	622	XAT	C18-C5-C6	-2.00	118.91	122.26
31	S	613	CLA	C1D-ND-C4D	-2.00	104.91	106.33
33	C	515	BCR	C37-C22-C21	-2.00	120.12	122.92
50	g1	623	NEX	C20-C13-C14	-2.00	120.12	122.92
31	B1	615	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (694) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	405	CLA	ND
31	A	406	CLA	ND
31	A	407	CLA	ND
31	A	410	CLA	ND
31	B	602	CLA	ND
31	B	603	CLA	ND
31	B	604	CLA	ND
31	B	605	CLA	ND
31	B	606	CLA	ND
31	B	607	CLA	ND
31	B	608	CLA	ND
31	B	609	CLA	ND
31	B	610	CLA	ND
31	B	611	CLA	ND
31	B	612	CLA	ND
31	B	613	CLA	ND
31	B	614	CLA	ND
31	B	615	CLA	ND
31	B	616	CLA	ND
31	B	617	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	C	501	CLA	ND
31	C	502	CLA	ND
31	C	503	CLA	ND
31	C	504	CLA	ND
31	C	505	CLA	ND
31	C	506	CLA	ND
31	C	507	CLA	ND
31	C	508	CLA	ND
31	C	509	CLA	ND
31	C	510	CLA	ND
31	C	511	CLA	ND
31	C	512	CLA	ND
31	C	513	CLA	ND
31	D	402	CLA	ND
31	D	403	CLA	ND
31	N	602	CLA	ND
31	N	603	CLA	ND
31	N	604	CLA	ND
31	N	610	CLA	ND
31	N	611	CLA	ND
31	N	612	CLA	ND
31	N	613	CLA	ND
31	N	614	CLA	ND
31	G	602	CLA	ND
31	G	603	CLA	ND
31	G	604	CLA	ND
31	G	610	CLA	ND
31	G	611	CLA	ND
31	G	612	CLA	ND
31	G	613	CLA	ND
31	G	614	CLA	ND
31	R	602	CLA	ND
31	R	603	CLA	ND
31	R	604	CLA	ND
31	R	608	CLA	ND
31	R	609	CLA	ND
31	R	610	CLA	ND
31	R	611	CLA	ND
31	R	612	CLA	ND
31	R	613	CLA	ND
31	S	602	CLA	ND
31	S	603	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	S	604	CLA	ND
31	S	605	CLA	ND
31	S	609	CLA	ND
31	S	610	CLA	ND
31	S	611	CLA	ND
31	S	612	CLA	ND
31	S	613	CLA	ND
31	S	614	CLA	ND
31	S	617	CLA	ND
31	Y	602	CLA	ND
31	Y	603	CLA	ND
31	Y	604	CLA	ND
31	Y	608	CLA	ND
31	Y	610	CLA	ND
31	Y	611	CLA	ND
31	Y	612	CLA	ND
31	Y	613	CLA	ND
31	Y	614	CLA	ND
31	a	405	CLA	ND
31	a	406	CLA	ND
31	a	407	CLA	ND
31	a	410	CLA	ND
31	b	602	CLA	ND
31	b	603	CLA	ND
31	b	604	CLA	ND
31	b	605	CLA	ND
31	b	606	CLA	ND
31	b	607	CLA	ND
31	b	608	CLA	ND
31	b	609	CLA	ND
31	b	610	CLA	ND
31	b	611	CLA	ND
31	b	612	CLA	ND
31	b	613	CLA	ND
31	b	614	CLA	ND
31	b	615	CLA	ND
31	b	616	CLA	ND
31	b	617	CLA	ND
31	c	501	CLA	ND
31	c	502	CLA	ND
31	c	503	CLA	ND
31	c	504	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	c	505	CLA	ND
31	c	506	CLA	ND
31	c	507	CLA	ND
31	c	508	CLA	ND
31	c	509	CLA	ND
31	c	510	CLA	ND
31	c	511	CLA	ND
31	c	512	CLA	ND
31	c	513	CLA	ND
31	d	402	CLA	ND
31	d	403	CLA	ND
31	n	602	CLA	ND
31	n	603	CLA	ND
31	n	604	CLA	ND
31	n	610	CLA	ND
31	n	611	CLA	ND
31	n	612	CLA	ND
31	n	613	CLA	ND
31	n	614	CLA	ND
31	g	602	CLA	ND
31	g	603	CLA	ND
31	g	604	CLA	ND
31	g	610	CLA	ND
31	g	611	CLA	ND
31	g	612	CLA	ND
31	g	613	CLA	ND
31	g	614	CLA	ND
31	r	602	CLA	ND
31	r	603	CLA	ND
31	r	604	CLA	ND
31	r	608	CLA	ND
31	r	609	CLA	ND
31	r	610	CLA	ND
31	r	611	CLA	ND
31	r	612	CLA	ND
31	r	613	CLA	ND
31	s	602	CLA	ND
31	s	603	CLA	ND
31	s	604	CLA	ND
31	s	605	CLA	ND
31	s	609	CLA	ND
31	s	610	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	s	611	CLA	ND
31	s	612	CLA	ND
31	s	613	CLA	ND
31	s	614	CLA	ND
31	s	617	CLA	ND
31	y	602	CLA	ND
31	y	603	CLA	ND
31	y	604	CLA	ND
31	y	608	CLA	ND
31	y	610	CLA	ND
31	y	611	CLA	ND
31	y	612	CLA	ND
31	y	613	CLA	ND
31	y	614	CLA	ND
31	A1	405	CLA	ND
31	A1	406	CLA	ND
31	A1	407	CLA	ND
31	A1	410	CLA	ND
31	B1	602	CLA	ND
31	B1	603	CLA	ND
31	B1	604	CLA	ND
31	B1	605	CLA	ND
31	B1	606	CLA	ND
31	B1	607	CLA	ND
31	B1	608	CLA	ND
31	B1	609	CLA	ND
31	B1	610	CLA	ND
31	B1	611	CLA	ND
31	B1	612	CLA	ND
31	B1	613	CLA	ND
31	B1	614	CLA	ND
31	B1	615	CLA	ND
31	B1	616	CLA	ND
31	B1	617	CLA	ND
31	C1	501	CLA	ND
31	C1	502	CLA	ND
31	C1	503	CLA	ND
31	C1	504	CLA	ND
31	C1	505	CLA	ND
31	C1	506	CLA	ND
31	C1	507	CLA	ND
31	C1	508	CLA	ND

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	C1	509	CLA	ND
31	C1	510	CLA	ND
31	C1	511	CLA	ND
31	C1	512	CLA	ND
31	C1	513	CLA	ND
31	D1	402	CLA	ND
31	D1	403	CLA	ND
31	N1	602	CLA	ND
31	N1	603	CLA	ND
31	N1	604	CLA	ND
31	N1	610	CLA	ND
31	N1	611	CLA	ND
31	N1	612	CLA	ND
31	N1	613	CLA	ND
31	N1	614	CLA	ND
31	G1	602	CLA	ND
31	G1	603	CLA	ND
31	G1	604	CLA	ND
31	G1	610	CLA	ND
31	G1	611	CLA	ND
31	G1	612	CLA	ND
31	G1	613	CLA	ND
31	G1	614	CLA	ND
31	R1	602	CLA	ND
31	R1	603	CLA	ND
31	R1	604	CLA	ND
31	R1	608	CLA	ND
31	R1	609	CLA	ND
31	R1	610	CLA	ND
31	R1	612	CLA	ND
31	S1	602	CLA	ND
31	S1	603	CLA	ND
31	S1	604	CLA	ND
31	S1	605	CLA	ND
31	S1	609	CLA	ND
31	S1	610	CLA	ND
31	S1	611	CLA	ND
31	S1	612	CLA	ND
31	S1	613	CLA	ND
31	S1	614	CLA	ND
31	S1	617	CLA	ND
31	Y1	602	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	Y1	603	CLA	ND
31	Y1	604	CLA	ND
31	Y1	608	CLA	ND
31	Y1	610	CLA	ND
31	Y1	611	CLA	ND
31	Y1	612	CLA	ND
31	Y1	613	CLA	ND
31	Y1	614	CLA	ND
31	a1	405	CLA	ND
31	a1	406	CLA	ND
31	a1	407	CLA	ND
31	a1	410	CLA	ND
31	b1	602	CLA	ND
31	b1	603	CLA	ND
31	b1	604	CLA	ND
31	b1	605	CLA	ND
31	b1	606	CLA	ND
31	b1	607	CLA	ND
31	b1	608	CLA	ND
31	b1	609	CLA	ND
31	b1	610	CLA	ND
31	b1	611	CLA	ND
31	b1	612	CLA	ND
31	b1	613	CLA	ND
31	b1	614	CLA	ND
31	b1	615	CLA	ND
31	b1	616	CLA	ND
31	b1	617	CLA	ND
31	c1	501	CLA	ND
31	c1	502	CLA	ND
31	c1	503	CLA	ND
31	c1	504	CLA	ND
31	c1	505	CLA	ND
31	c1	506	CLA	ND
31	c1	507	CLA	ND
31	c1	508	CLA	ND
31	c1	509	CLA	ND
31	c1	510	CLA	ND
31	c1	511	CLA	ND
31	c1	512	CLA	ND
31	c1	513	CLA	ND
31	d1	402	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	d1	403	CLA	ND
31	n1	602	CLA	ND
31	n1	603	CLA	ND
31	n1	604	CLA	ND
31	n1	610	CLA	ND
31	n1	611	CLA	ND
31	n1	612	CLA	ND
31	n1	613	CLA	ND
31	n1	614	CLA	ND
31	g1	602	CLA	ND
31	g1	603	CLA	ND
31	g1	604	CLA	ND
31	g1	610	CLA	ND
31	g1	611	CLA	ND
31	g1	612	CLA	ND
31	g1	613	CLA	ND
31	g1	614	CLA	ND
31	r1	602	CLA	ND
31	r1	603	CLA	ND
31	r1	604	CLA	ND
31	r1	608	CLA	ND
31	r1	609	CLA	ND
31	r1	610	CLA	ND
31	r1	612	CLA	ND
31	s1	602	CLA	ND
31	s1	603	CLA	ND
31	s1	604	CLA	ND
31	s1	605	CLA	ND
31	s1	609	CLA	ND
31	s1	610	CLA	ND
31	s1	611	CLA	ND
31	s1	612	CLA	ND
31	s1	613	CLA	ND
31	s1	614	CLA	ND
31	s1	617	CLA	ND
31	y1	602	CLA	ND
31	y1	603	CLA	ND
31	y1	604	CLA	ND
31	y1	608	CLA	ND
31	y1	610	CLA	ND
31	y1	611	CLA	ND
31	y1	612	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	y1	613	CLA	ND
31	y1	614	CLA	ND
37	B	620	C7Z	C3
37	b	620	C7Z	C3
37	B1	620	C7Z	C3
37	b1	620	C7Z	C3
42	C	527	LMK	C3
42	c	627	LMK	C3
42	C1	527	LMK	C3
42	C1	527	LMK	C8
42	c1	527	LMK	C3
42	c1	527	LMK	C8
46	H	101	RRX	C28
46	h	101	RRX	C28
46	H1	101	RRX	C28
46	h1	101	RRX	C28
47	N	601	CHL	NA
47	N	601	CHL	C8
47	N	601	CHL	ND
47	N	601	CHL	NC
47	N	605	CHL	NA
47	N	605	CHL	C8
47	N	605	CHL	ND
47	N	605	CHL	NC
47	N	606	CHL	NA
47	N	606	CHL	C8
47	N	606	CHL	ND
47	N	606	CHL	NC
47	N	607	CHL	NA
47	N	607	CHL	C8
47	N	607	CHL	ND
47	N	607	CHL	NC
47	N	608	CHL	NA
47	N	608	CHL	ND
47	N	608	CHL	NC
47	N	609	CHL	NA
47	N	609	CHL	C8
47	N	609	CHL	ND
47	N	609	CHL	NC
47	G	601	CHL	NA
47	G	601	CHL	C8
47	G	601	CHL	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
47	G	601	CHL	NC
47	G	605	CHL	NA
47	G	605	CHL	ND
47	G	605	CHL	NC
47	G	606	CHL	NA
47	G	606	CHL	ND
47	G	606	CHL	NC
47	G	606	CHL	C3A
47	G	607	CHL	NA
47	G	607	CHL	ND
47	G	607	CHL	NC
47	G	608	CHL	NA
47	G	608	CHL	ND
47	G	608	CHL	NC
47	G	609	CHL	NA
47	G	609	CHL	C8
47	G	609	CHL	ND
47	G	609	CHL	NC
47	R	606	CHL	NA
47	R	606	CHL	ND
47	R	606	CHL	NC
47	R	607	CHL	NA
47	R	607	CHL	ND
47	R	607	CHL	NC
47	S	601	CHL	NA
47	S	601	CHL	ND
47	S	601	CHL	NC
47	S	606	CHL	NA
47	S	606	CHL	ND
47	S	606	CHL	NC
47	S	607	CHL	NA
47	S	607	CHL	ND
47	S	607	CHL	NC
47	S	607	CHL	C3A
47	S	608	CHL	NA
47	S	608	CHL	C8
47	S	608	CHL	ND
47	S	608	CHL	NC
47	Y	601	CHL	NA
47	Y	601	CHL	C8
47	Y	601	CHL	ND
47	Y	601	CHL	NC

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
47	Y	605	CHL	NA
47	Y	605	CHL	ND
47	Y	605	CHL	NC
47	Y	606	CHL	NA
47	Y	606	CHL	C8
47	Y	606	CHL	ND
47	Y	606	CHL	NC
47	Y	607	CHL	NA
47	Y	607	CHL	C8
47	Y	607	CHL	ND
47	Y	607	CHL	NC
47	Y	609	CHL	NA
47	Y	609	CHL	C8
47	Y	609	CHL	ND
47	Y	609	CHL	NC
47	n	601	CHL	NA
47	n	601	CHL	C8
47	n	601	CHL	ND
47	n	601	CHL	NC
47	n	605	CHL	NA
47	n	605	CHL	C8
47	n	605	CHL	ND
47	n	605	CHL	NC
47	n	606	CHL	NA
47	n	606	CHL	C8
47	n	606	CHL	ND
47	n	606	CHL	NC
47	n	607	CHL	NA
47	n	607	CHL	C8
47	n	607	CHL	ND
47	n	607	CHL	NC
47	n	608	CHL	NA
47	n	608	CHL	ND
47	n	608	CHL	NC
47	n	609	CHL	NA
47	n	609	CHL	C8
47	n	609	CHL	ND
47	n	609	CHL	NC
47	g	601	CHL	NA
47	g	601	CHL	C8
47	g	601	CHL	ND
47	g	601	CHL	NC

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
47	g	605	CHL	NA
47	g	605	CHL	ND
47	g	605	CHL	NC
47	g	606	CHL	NA
47	g	606	CHL	ND
47	g	606	CHL	NC
47	g	607	CHL	NA
47	g	607	CHL	ND
47	g	607	CHL	NC
47	g	608	CHL	NA
47	g	608	CHL	ND
47	g	608	CHL	NC
47	g	609	CHL	NA
47	g	609	CHL	C8
47	g	609	CHL	ND
47	g	609	CHL	NC
47	r	606	CHL	NA
47	r	606	CHL	ND
47	r	606	CHL	NC
47	r	607	CHL	NA
47	r	607	CHL	ND
47	r	607	CHL	NC
47	s	601	CHL	NA
47	s	601	CHL	ND
47	s	601	CHL	NC
47	s	606	CHL	NA
47	s	606	CHL	ND
47	s	606	CHL	NC
47	s	607	CHL	NA
47	s	607	CHL	ND
47	s	607	CHL	NC
47	s	607	CHL	C3A
47	s	608	CHL	NA
47	s	608	CHL	C8
47	s	608	CHL	ND
47	s	608	CHL	NC
47	y	601	CHL	NA
47	y	601	CHL	C8
47	y	601	CHL	ND
47	y	601	CHL	NC
47	y	605	CHL	NA
47	y	605	CHL	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
47	y	605	CHL	NC
47	y	606	CHL	NA
47	y	606	CHL	C8
47	y	606	CHL	ND
47	y	606	CHL	NC
47	y	607	CHL	NA
47	y	607	CHL	C8
47	y	607	CHL	ND
47	y	607	CHL	NC
47	y	609	CHL	NA
47	y	609	CHL	C8
47	y	609	CHL	ND
47	y	609	CHL	NC
47	N1	601	CHL	NA
47	N1	601	CHL	C8
47	N1	601	CHL	ND
47	N1	601	CHL	NC
47	N1	605	CHL	NA
47	N1	605	CHL	C8
47	N1	605	CHL	ND
47	N1	605	CHL	NC
47	N1	606	CHL	NA
47	N1	606	CHL	C8
47	N1	606	CHL	ND
47	N1	606	CHL	NC
47	N1	607	CHL	NA
47	N1	607	CHL	C8
47	N1	607	CHL	ND
47	N1	607	CHL	NC
47	N1	608	CHL	NA
47	N1	608	CHL	ND
47	N1	608	CHL	NC
47	N1	609	CHL	NA
47	N1	609	CHL	C8
47	N1	609	CHL	ND
47	N1	609	CHL	NC
47	G1	601	CHL	NA
47	G1	601	CHL	C8
47	G1	601	CHL	ND
47	G1	601	CHL	NC
47	G1	605	CHL	NA
47	G1	605	CHL	ND

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
47	G1	605	CHL	NC
47	G1	605	CHL	C3A
47	G1	606	CHL	NA
47	G1	606	CHL	ND
47	G1	606	CHL	NC
47	G1	607	CHL	NA
47	G1	607	CHL	C8
47	G1	607	CHL	ND
47	G1	607	CHL	NC
47	G1	608	CHL	NA
47	G1	608	CHL	ND
47	G1	608	CHL	NC
47	G1	609	CHL	NA
47	G1	609	CHL	C8
47	G1	609	CHL	ND
47	G1	609	CHL	NC
47	R1	606	CHL	NA
47	R1	606	CHL	ND
47	R1	606	CHL	NC
47	R1	607	CHL	NA
47	R1	607	CHL	ND
47	R1	607	CHL	NC
47	S1	601	CHL	NA
47	S1	601	CHL	ND
47	S1	601	CHL	NC
47	S1	606	CHL	NA
47	S1	606	CHL	ND
47	S1	606	CHL	NC
47	S1	607	CHL	NA
47	S1	607	CHL	ND
47	S1	607	CHL	NC
47	S1	608	CHL	NA
47	S1	608	CHL	C8
47	S1	608	CHL	ND
47	S1	608	CHL	NC
47	Y1	601	CHL	NA
47	Y1	601	CHL	C8
47	Y1	601	CHL	ND
47	Y1	601	CHL	NC
47	Y1	605	CHL	NA
47	Y1	605	CHL	ND
47	Y1	605	CHL	NC

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
47	Y1	606	CHL	NA
47	Y1	606	CHL	C8
47	Y1	606	CHL	ND
47	Y1	606	CHL	NC
47	Y1	607	CHL	NA
47	Y1	607	CHL	C8
47	Y1	607	CHL	ND
47	Y1	607	CHL	NC
47	Y1	609	CHL	NA
47	Y1	609	CHL	C8
47	Y1	609	CHL	ND
47	Y1	609	CHL	NC
47	n1	601	CHL	NA
47	n1	601	CHL	C8
47	n1	601	CHL	ND
47	n1	601	CHL	NC
47	n1	605	CHL	NA
47	n1	605	CHL	C8
47	n1	605	CHL	ND
47	n1	605	CHL	NC
47	n1	606	CHL	NA
47	n1	606	CHL	C8
47	n1	606	CHL	ND
47	n1	606	CHL	NC
47	n1	607	CHL	NA
47	n1	607	CHL	C8
47	n1	607	CHL	ND
47	n1	607	CHL	NC
47	n1	608	CHL	NA
47	n1	608	CHL	ND
47	n1	608	CHL	NC
47	n1	609	CHL	NA
47	n1	609	CHL	C8
47	n1	609	CHL	ND
47	n1	609	CHL	NC
47	g1	601	CHL	NA
47	g1	601	CHL	C8
47	g1	601	CHL	ND
47	g1	601	CHL	NC
47	g1	605	CHL	NA
47	g1	605	CHL	ND
47	g1	605	CHL	NC

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
47	g1	605	CHL	C3A
47	g1	606	CHL	NA
47	g1	606	CHL	ND
47	g1	606	CHL	NC
47	g1	607	CHL	NA
47	g1	607	CHL	C8
47	g1	607	CHL	ND
47	g1	607	CHL	NC
47	g1	608	CHL	NA
47	g1	608	CHL	ND
47	g1	608	CHL	NC
47	g1	609	CHL	NA
47	g1	609	CHL	C8
47	g1	609	CHL	ND
47	g1	609	CHL	NC
47	r1	606	CHL	NA
47	r1	606	CHL	ND
47	r1	606	CHL	NC
47	r1	607	CHL	NA
47	r1	607	CHL	ND
47	r1	607	CHL	NC
47	s1	601	CHL	NA
47	s1	601	CHL	ND
47	s1	601	CHL	NC
47	s1	606	CHL	NA
47	s1	606	CHL	ND
47	s1	606	CHL	NC
47	s1	607	CHL	NA
47	s1	607	CHL	ND
47	s1	607	CHL	NC
47	s1	608	CHL	NA
47	s1	608	CHL	C8
47	s1	608	CHL	ND
47	s1	608	CHL	NC
47	y1	601	CHL	NA
47	y1	601	CHL	C8
47	y1	601	CHL	ND
47	y1	601	CHL	NC
47	y1	605	CHL	NA
47	y1	605	CHL	ND
47	y1	605	CHL	NC
47	y1	606	CHL	NA

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
47	y1	606	CHL	C8
47	y1	606	CHL	ND
47	y1	606	CHL	NC
47	y1	607	CHL	NA
47	y1	607	CHL	C8
47	y1	607	CHL	ND
47	y1	607	CHL	NC
47	y1	609	CHL	NA
47	y1	609	CHL	C8
47	y1	609	CHL	ND
47	y1	609	CHL	NC
48	G	621	LUT	C26
48	S	620	LUT	C26
48	Y	621	LUT	C26
48	n	621	LUT	C26
48	s	620	LUT	C26
48	R1	620	LUT	C26
48	g1	621	LUT	C26
49	N	622	XAT	C6
49	G	622	XAT	C6
49	G	622	XAT	C26
49	R	621	XAT	C26
49	Y	622	XAT	C6
49	g	622	XAT	C6
49	g	622	XAT	C26
49	r	622	XAT	C26
49	N1	622	XAT	C6
49	G1	622	XAT	C26
49	Y1	622	XAT	C6
49	Y1	622	XAT	C26
49	n1	622	XAT	C6
49	g1	622	XAT	C6
49	g1	622	XAT	C26
49	r1	621	XAT	C26
56	R1	626	ERG	C14
56	R1	626	ERG	C9
56	R1	626	ERG	C24
56	R1	626	ERG	C10
56	R1	626	ERG	C20
56	r1	626	ERG	C14
56	r1	626	ERG	C9
56	r1	626	ERG	C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
56	r1	626	ERG	C10
56	r1	626	ERG	C20

All (8670) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	405	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C3A-C2A-CAA-CBA
31	A	406	CLA	CHA-CBD-CGD-O1D
31	A	406	CLA	CHA-CBD-CGD-O2D
31	A	407	CLA	CHA-CBD-CGD-O1D
31	A	407	CLA	CHA-CBD-CGD-O2D
31	B	602	CLA	CHA-CBD-CGD-O1D
31	B	602	CLA	CHA-CBD-CGD-O2D
31	B	602	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	CHA-CBD-CGD-O1D
31	B	603	CLA	CHA-CBD-CGD-O2D
31	B	604	CLA	CBD-CGD-O2D-CED
31	B	605	CLA	C2-C1-O2A-CGA
31	B	605	CLA	CHA-CBD-CGD-O1D
31	B	605	CLA	CHA-CBD-CGD-O2D
31	B	605	CLA	CAD-CBD-CGD-O1D
31	B	605	CLA	C2-C3-C5-C6
31	B	605	CLA	C4-C3-C5-C6
31	B	606	CLA	C2-C3-C5-C6
31	B	606	CLA	C4-C3-C5-C6
31	B	607	CLA	CHA-CBD-CGD-O1D
31	B	607	CLA	CHA-CBD-CGD-O2D
31	B	608	CLA	C1A-C2A-CAA-CBA
31	B	608	CLA	C3A-C2A-CAA-CBA
31	B	608	CLA	C2-C1-O2A-CGA
31	B	608	CLA	CAD-CBD-CGD-O1D
31	B	608	CLA	CAD-CBD-CGD-O2D
31	B	608	CLA	CBD-CGD-O2D-CED
31	B	608	CLA	C2-C3-C5-C6
31	B	608	CLA	C4-C3-C5-C6
31	B	609	CLA	C1A-C2A-CAA-CBA
31	B	610	CLA	C1A-C2A-CAA-CBA
31	B	610	CLA	C3A-C2A-CAA-CBA
31	B	610	CLA	CHA-CBD-CGD-O1D
31	B	610	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B	610	CLA	CBD-CGD-O2D-CED
31	B	612	CLA	C1A-C2A-CAA-CBA
31	B	612	CLA	C2-C1-O2A-CGA
31	B	612	CLA	C2-C3-C5-C6
31	B	612	CLA	C4-C3-C5-C6
31	B	614	CLA	C2-C1-O2A-CGA
31	B	615	CLA	C1A-C2A-CAA-CBA
31	B	615	CLA	CHA-CBD-CGD-O1D
31	B	615	CLA	CHA-CBD-CGD-O2D
31	B	615	CLA	CAD-CBD-CGD-O1D
31	B	615	CLA	CAD-CBD-CGD-O2D
31	C	501	CLA	C2-C3-C5-C6
31	C	501	CLA	C4-C3-C5-C6
31	C	502	CLA	CHA-CBD-CGD-O1D
31	C	502	CLA	CHA-CBD-CGD-O2D
31	C	502	CLA	CAD-CBD-CGD-O1D
31	C	502	CLA	CAD-CBD-CGD-O2D
31	C	503	CLA	C2-C3-C5-C6
31	C	503	CLA	C4-C3-C5-C6
31	C	504	CLA	C2-C3-C5-C6
31	C	504	CLA	C4-C3-C5-C6
31	C	505	CLA	CHA-CBD-CGD-O1D
31	C	505	CLA	CHA-CBD-CGD-O2D
31	C	505	CLA	CAD-CBD-CGD-O1D
31	C	508	CLA	CHA-CBD-CGD-O1D
31	C	508	CLA	CHA-CBD-CGD-O2D
31	C	511	CLA	CHA-CBD-CGD-O1D
31	C	511	CLA	CHA-CBD-CGD-O2D
31	C	512	CLA	CHA-CBD-CGD-O1D
31	C	512	CLA	CHA-CBD-CGD-O2D
31	C	513	CLA	C1A-C2A-CAA-CBA
31	C	513	CLA	C11-C10-C8-C9
31	D	402	CLA	C1A-C2A-CAA-CBA
31	D	402	CLA	CBD-CGD-O2D-CED
31	D	402	CLA	C2-C3-C5-C6
31	D	402	CLA	C4-C3-C5-C6
31	D	403	CLA	CBD-CGD-O2D-CED
31	N	602	CLA	C14-C13-C15-C16
31	N	603	CLA	C3A-C2A-CAA-CBA
31	N	610	CLA	C1A-C2A-CAA-CBA
31	N	611	CLA	CHA-CBD-CGD-O1D
31	N	611	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N	613	CLA	C1A-C2A-CAA-CBA
31	N	613	CLA	CHA-CBD-CGD-O1D
31	N	613	CLA	CHA-CBD-CGD-O2D
31	N	614	CLA	CBD-CGD-O2D-CED
31	G	602	CLA	C1A-C2A-CAA-CBA
31	G	602	CLA	C3A-C2A-CAA-CBA
31	G	603	CLA	CBD-CGD-O2D-CED
31	G	610	CLA	CHA-CBD-CGD-O1D
31	G	610	CLA	CHA-CBD-CGD-O2D
31	G	614	CLA	CBD-CGD-O2D-CED
31	R	602	CLA	CHA-CBD-CGD-O1D
31	R	602	CLA	CHA-CBD-CGD-O2D
31	R	603	CLA	C2-C1-O2A-CGA
31	R	608	CLA	C3A-C2A-CAA-CBA
31	R	608	CLA	CBD-CGD-O2D-CED
31	R	610	CLA	C1A-C2A-CAA-CBA
31	R	610	CLA	CHA-CBD-CGD-O1D
31	R	610	CLA	CHA-CBD-CGD-O2D
31	R	610	CLA	C2-C3-C5-C6
31	R	610	CLA	C4-C3-C5-C6
31	R	611	CLA	CBA-CGA-O2A-C1
31	R	611	CLA	O1A-CGA-O2A-C1
31	R	611	CLA	CBD-CGD-O2D-CED
31	R	612	CLA	C2-C1-O2A-CGA
31	R	613	CLA	CBA-CGA-O2A-C1
31	S	602	CLA	C1A-C2A-CAA-CBA
31	S	602	CLA	C3A-C2A-CAA-CBA
31	S	602	CLA	CHA-CBD-CGD-O1D
31	S	602	CLA	CHA-CBD-CGD-O2D
31	S	605	CLA	C1A-C2A-CAA-CBA
31	S	605	CLA	C3A-C2A-CAA-CBA
31	S	605	CLA	C2-C1-O2A-CGA
31	S	605	CLA	CHA-CBD-CGD-O1D
31	S	605	CLA	CHA-CBD-CGD-O2D
31	S	609	CLA	CBD-CGD-O2D-CED
31	S	610	CLA	CHA-CBD-CGD-O1D
31	S	610	CLA	CHA-CBD-CGD-O2D
31	S	611	CLA	CBD-CGD-O2D-CED
31	S	617	CLA	C2A-CAA-CBA-CGA
31	S	617	CLA	CBA-CGA-O2A-C1
31	S	617	CLA	O1A-CGA-O2A-C1
31	S	617	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	S	617	CLA	CHA-CBD-CGD-O2D
31	Y	604	CLA	CHA-CBD-CGD-O1D
31	Y	604	CLA	CHA-CBD-CGD-O2D
31	Y	613	CLA	CHA-CBD-CGD-O1D
31	Y	613	CLA	CHA-CBD-CGD-O2D
31	Y	613	CLA	CBD-CGD-O2D-CED
31	Y	614	CLA	CBD-CGD-O2D-CED
31	a	405	CLA	CBD-CGD-O2D-CED
31	a	406	CLA	C1A-C2A-CAA-CBA
31	a	406	CLA	C3A-C2A-CAA-CBA
31	a	406	CLA	CHA-CBD-CGD-O1D
31	a	406	CLA	CHA-CBD-CGD-O2D
31	a	407	CLA	CHA-CBD-CGD-O1D
31	a	407	CLA	CHA-CBD-CGD-O2D
31	a	410	CLA	CHA-CBD-CGD-O1D
31	a	410	CLA	CHA-CBD-CGD-O2D
31	b	603	CLA	CHA-CBD-CGD-O1D
31	b	603	CLA	CHA-CBD-CGD-O2D
31	b	604	CLA	CBD-CGD-O2D-CED
31	b	605	CLA	C2-C1-O2A-CGA
31	b	605	CLA	CHA-CBD-CGD-O1D
31	b	605	CLA	CHA-CBD-CGD-O2D
31	b	607	CLA	C1A-C2A-CAA-CBA
31	b	607	CLA	C4-C3-C5-C6
31	b	608	CLA	C1A-C2A-CAA-CBA
31	b	608	CLA	C3A-C2A-CAA-CBA
31	b	608	CLA	CHA-CBD-CGD-O1D
31	b	608	CLA	CHA-CBD-CGD-O2D
31	b	608	CLA	CAD-CBD-CGD-O1D
31	b	608	CLA	C2-C3-C5-C6
31	b	608	CLA	C4-C3-C5-C6
31	b	609	CLA	C1A-C2A-CAA-CBA
31	b	609	CLA	CHA-CBD-CGD-O1D
31	b	609	CLA	CHA-CBD-CGD-O2D
31	b	610	CLA	C3A-C2A-CAA-CBA
31	b	610	CLA	CHA-CBD-CGD-O1D
31	b	610	CLA	CBD-CGD-O2D-CED
31	b	612	CLA	C1A-C2A-CAA-CBA
31	b	612	CLA	CBD-CGD-O2D-CED
31	b	612	CLA	C4-C3-C5-C6
31	b	615	CLA	C1A-C2A-CAA-CBA
31	b	615	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b	615	CLA	CAD-CBD-CGD-O2D
31	b	616	CLA	CHA-CBD-CGD-O1D
31	b	616	CLA	CHA-CBD-CGD-O2D
31	b	617	CLA	CBA-CGA-O2A-C1
31	b	617	CLA	O1A-CGA-O2A-C1
31	b	617	CLA	C6-C7-C8-C9
31	c	501	CLA	C1A-C2A-CAA-CBA
31	c	501	CLA	CHA-CBD-CGD-O2D
31	c	502	CLA	CBD-CGD-O2D-CED
31	c	504	CLA	CBA-CGA-O2A-C1
31	c	504	CLA	O1A-CGA-O2A-C1
31	c	505	CLA	CHA-CBD-CGD-O1D
31	c	505	CLA	CAD-CBD-CGD-O1D
31	c	505	CLA	CAD-CBD-CGD-O2D
31	c	506	CLA	C6-C7-C8-C9
31	c	508	CLA	CHA-CBD-CGD-O1D
31	c	508	CLA	CHA-CBD-CGD-O2D
31	c	512	CLA	CHA-CBD-CGD-O1D
31	c	512	CLA	CHA-CBD-CGD-O2D
31	c	512	CLA	C2-C3-C5-C6
31	c	512	CLA	C4-C3-C5-C6
31	d	402	CLA	C4-C3-C5-C6
31	d	403	CLA	CBD-CGD-O2D-CED
31	n	603	CLA	C1A-C2A-CAA-CBA
31	n	603	CLA	C2A-CAA-CBA-CGA
31	n	603	CLA	CBA-CGA-O2A-C1
31	n	603	CLA	O1A-CGA-O2A-C1
31	n	603	CLA	CHA-CBD-CGD-O1D
31	n	603	CLA	CHA-CBD-CGD-O2D
31	n	603	CLA	CAD-CBD-CGD-O1D
31	n	603	CLA	CBD-CGD-O2D-CED
31	n	604	CLA	C1A-C2A-CAA-CBA
31	n	604	CLA	C3A-C2A-CAA-CBA
31	n	610	CLA	C1A-C2A-CAA-CBA
31	n	610	CLA	CBD-CGD-O2D-CED
31	n	611	CLA	C1A-C2A-CAA-CBA
31	n	611	CLA	C3A-C2A-CAA-CBA
31	n	611	CLA	CHA-CBD-CGD-O1D
31	n	611	CLA	CHA-CBD-CGD-O2D
31	n	612	CLA	CBD-CGD-O2D-CED
31	n	614	CLA	C1A-C2A-CAA-CBA
31	n	614	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	g	602	CLA	C1A-C2A-CAA-CBA
31	g	602	CLA	C3A-C2A-CAA-CBA
31	g	603	CLA	C3A-C2A-CAA-CBA
31	g	603	CLA	CBD-CGD-O2D-CED
31	g	604	CLA	C2-C1-O2A-CGA
31	g	604	CLA	CBD-CGD-O2D-CED
31	g	610	CLA	CHA-CBD-CGD-O1D
31	g	610	CLA	CHA-CBD-CGD-O2D
31	g	612	CLA	C1A-C2A-CAA-CBA
31	g	612	CLA	CHA-CBD-CGD-O1D
31	g	612	CLA	CHA-CBD-CGD-O2D
31	r	603	CLA	C2-C1-O2A-CGA
31	r	603	CLA	CBD-CGD-O2D-CED
31	r	604	CLA	C1A-C2A-CAA-CBA
31	r	604	CLA	C3A-C2A-CAA-CBA
31	r	608	CLA	C1A-C2A-CAA-CBA
31	r	608	CLA	C3A-C2A-CAA-CBA
31	r	609	CLA	C2A-CAA-CBA-CGA
31	r	609	CLA	CHA-CBD-CGD-O1D
31	r	609	CLA	CHA-CBD-CGD-O2D
31	r	609	CLA	CBD-CGD-O2D-CED
31	r	610	CLA	C1A-C2A-CAA-CBA
31	r	610	CLA	CHA-CBD-CGD-O1D
31	r	610	CLA	CHA-CBD-CGD-O2D
31	r	610	CLA	C2-C3-C5-C6
31	r	610	CLA	C4-C3-C5-C6
31	r	611	CLA	CBA-CGA-O2A-C1
31	r	612	CLA	C2-C1-O2A-CGA
31	r	613	CLA	CBA-CGA-O2A-C1
31	r	613	CLA	O1A-CGA-O2A-C1
31	s	602	CLA	C1A-C2A-CAA-CBA
31	s	602	CLA	C3A-C2A-CAA-CBA
31	s	602	CLA	CHA-CBD-CGD-O1D
31	s	602	CLA	CHA-CBD-CGD-O2D
31	s	603	CLA	CBD-CGD-O2D-CED
31	s	603	CLA	C2-C3-C5-C6
31	s	603	CLA	C4-C3-C5-C6
31	s	604	CLA	CHA-CBD-CGD-O1D
31	s	604	CLA	CHA-CBD-CGD-O2D
31	s	604	CLA	CBD-CGD-O2D-CED
31	s	605	CLA	C1A-C2A-CAA-CBA
31	s	605	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s	605	CLA	CHA-CBD-CGD-O2D
31	s	610	CLA	C1A-C2A-CAA-CBA
31	s	610	CLA	CHA-CBD-CGD-O1D
31	s	610	CLA	CHA-CBD-CGD-O2D
31	s	610	CLA	CBD-CGD-O2D-CED
31	s	611	CLA	CBD-CGD-O2D-CED
31	s	612	CLA	CBD-CGD-O2D-CED
31	s	613	CLA	CHA-CBD-CGD-O2D
31	s	614	CLA	CBA-CGA-O2A-C1
31	s	614	CLA	O1A-CGA-O2A-C1
31	y	602	CLA	CHA-CBD-CGD-O1D
31	y	602	CLA	CHA-CBD-CGD-O2D
31	y	610	CLA	CHA-CBD-CGD-O1D
31	y	610	CLA	CHA-CBD-CGD-O2D
31	y	613	CLA	CHA-CBD-CGD-O1D
31	y	613	CLA	CHA-CBD-CGD-O2D
31	y	614	CLA	C2-C1-O2A-CGA
31	A1	405	CLA	C3A-C2A-CAA-CBA
31	A1	405	CLA	CBD-CGD-O2D-CED
31	A1	406	CLA	C1A-C2A-CAA-CBA
31	A1	406	CLA	C3A-C2A-CAA-CBA
31	A1	406	CLA	C2-C1-O2A-CGA
31	A1	406	CLA	CHA-CBD-CGD-O1D
31	A1	406	CLA	CHA-CBD-CGD-O2D
31	A1	407	CLA	C2-C1-O2A-CGA
31	B1	602	CLA	C1A-C2A-CAA-CBA
31	B1	602	CLA	C2-C1-O2A-CGA
31	B1	602	CLA	CAD-CBD-CGD-O1D
31	B1	602	CLA	CAD-CBD-CGD-O2D
31	B1	603	CLA	CHA-CBD-CGD-O1D
31	B1	603	CLA	CBD-CGD-O2D-CED
31	B1	604	CLA	C2-C3-C5-C6
31	B1	604	CLA	C4-C3-C5-C6
31	B1	604	CLA	C11-C10-C8-C9
31	B1	605	CLA	CHA-CBD-CGD-O1D
31	B1	605	CLA	CAD-CBD-CGD-O1D
31	B1	605	CLA	CAD-CBD-CGD-O2D
31	B1	607	CLA	CHA-CBD-CGD-O1D
31	B1	607	CLA	CHA-CBD-CGD-O2D
31	B1	608	CLA	C1A-C2A-CAA-CBA
31	B1	608	CLA	C3A-C2A-CAA-CBA
31	B1	608	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B1	608	CLA	CHA-CBD-CGD-O2D
31	B1	608	CLA	CBD-CGD-O2D-CED
31	B1	608	CLA	C2-C3-C5-C6
31	B1	608	CLA	C4-C3-C5-C6
31	B1	609	CLA	C1A-C2A-CAA-CBA
31	B1	609	CLA	C3A-C2A-CAA-CBA
31	B1	609	CLA	CHA-CBD-CGD-O1D
31	B1	609	CLA	CHA-CBD-CGD-O2D
31	B1	610	CLA	CAD-CBD-CGD-O1D
31	B1	610	CLA	CAD-CBD-CGD-O2D
31	B1	610	CLA	CBD-CGD-O2D-CED
31	B1	612	CLA	CHA-CBD-CGD-O1D
31	B1	612	CLA	CHA-CBD-CGD-O2D
31	B1	613	CLA	C1A-C2A-CAA-CBA
31	B1	613	CLA	C3A-C2A-CAA-CBA
31	B1	613	CLA	C2-C1-O2A-CGA
31	B1	614	CLA	C2-C1-O2A-CGA
31	B1	614	CLA	CBD-CGD-O2D-CED
31	B1	615	CLA	C2-C3-C5-C6
31	B1	615	CLA	C4-C3-C5-C6
31	B1	616	CLA	CBD-CGD-O2D-CED
31	B1	616	CLA	C11-C10-C8-C9
31	B1	617	CLA	CBD-CGD-O2D-CED
31	C1	502	CLA	CHA-CBD-CGD-O1D
31	C1	503	CLA	CBD-CGD-O2D-CED
31	C1	504	CLA	CHA-CBD-CGD-O1D
31	C1	504	CLA	CHA-CBD-CGD-O2D
31	C1	504	CLA	CAD-CBD-CGD-O1D
31	C1	504	CLA	CAD-CBD-CGD-O2D
31	C1	505	CLA	CAD-CBD-CGD-O1D
31	C1	505	CLA	CAD-CBD-CGD-O2D
31	C1	506	CLA	C2-C1-O2A-CGA
31	C1	506	CLA	CHA-CBD-CGD-O1D
31	C1	506	CLA	CHA-CBD-CGD-O2D
31	C1	506	CLA	CAD-CBD-CGD-O1D
31	C1	506	CLA	CBD-CGD-O2D-CED
31	C1	508	CLA	CHA-CBD-CGD-O1D
31	C1	508	CLA	CHA-CBD-CGD-O2D
31	C1	509	CLA	C2-C1-O2A-CGA
31	C1	509	CLA	CBD-CGD-O2D-CED
31	C1	510	CLA	CBD-CGD-O2D-CED
31	C1	511	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C1	511	CLA	CHA-CBD-CGD-O2D
31	C1	512	CLA	C1A-C2A-CAA-CBA
31	C1	512	CLA	CBA-CGA-O2A-C1
31	C1	512	CLA	O1A-CGA-O2A-C1
31	C1	512	CLA	CBD-CGD-O2D-CED
31	C1	513	CLA	C1A-C2A-CAA-CBA
31	C1	513	CLA	C3A-C2A-CAA-CBA
31	C1	513	CLA	CBD-CGD-O2D-CED
31	C1	513	CLA	C11-C10-C8-C9
31	D1	402	CLA	CHA-CBD-CGD-O1D
31	D1	402	CLA	CHA-CBD-CGD-O2D
31	D1	402	CLA	CBD-CGD-O2D-CED
31	D1	402	CLA	C2-C3-C5-C6
31	D1	402	CLA	C4-C3-C5-C6
31	N1	602	CLA	CBD-CGD-O2D-CED
31	N1	603	CLA	CBD-CGD-O2D-CED
31	N1	604	CLA	C1A-C2A-CAA-CBA
31	N1	604	CLA	C3A-C2A-CAA-CBA
31	N1	604	CLA	C2A-CAA-CBA-CGA
31	N1	610	CLA	C1A-C2A-CAA-CBA
31	N1	610	CLA	C3A-C2A-CAA-CBA
31	N1	611	CLA	C2A-CAA-CBA-CGA
31	N1	611	CLA	C2-C1-O2A-CGA
31	N1	611	CLA	CHA-CBD-CGD-O1D
31	N1	611	CLA	CHA-CBD-CGD-O2D
31	N1	613	CLA	C1A-C2A-CAA-CBA
31	N1	614	CLA	C1A-C2A-CAA-CBA
31	N1	614	CLA	CBD-CGD-O2D-CED
31	G1	602	CLA	C1A-C2A-CAA-CBA
31	G1	602	CLA	C3A-C2A-CAA-CBA
31	G1	602	CLA	CBD-CGD-O2D-CED
31	G1	604	CLA	CBD-CGD-O2D-CED
31	G1	610	CLA	CBD-CGD-O2D-CED
31	G1	610	CLA	O1D-CGD-O2D-CED
31	G1	613	CLA	C2A-CAA-CBA-CGA
31	G1	614	CLA	CBA-CGA-O2A-C1
31	G1	614	CLA	CBD-CGD-O2D-CED
31	R1	602	CLA	CHA-CBD-CGD-O2D
31	R1	603	CLA	C2-C1-O2A-CGA
31	R1	603	CLA	CBD-CGD-O2D-CED
31	R1	604	CLA	C2-C1-O2A-CGA
31	R1	604	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R1	608	CLA	C1A-C2A-CAA-CBA
31	R1	608	CLA	C3A-C2A-CAA-CBA
31	R1	609	CLA	CHA-CBD-CGD-O1D
31	R1	609	CLA	CHA-CBD-CGD-O2D
31	R1	609	CLA	CBD-CGD-O2D-CED
31	R1	610	CLA	CHA-CBD-CGD-O1D
31	R1	610	CLA	CHA-CBD-CGD-O2D
31	R1	610	CLA	CBD-CGD-O2D-CED
31	R1	612	CLA	C1A-C2A-CAA-CBA
31	R1	612	CLA	C3A-C2A-CAA-CBA
31	R1	612	CLA	CBD-CGD-O2D-CED
31	S1	602	CLA	C2-C1-O2A-CGA
31	S1	603	CLA	C1A-C2A-CAA-CBA
31	S1	603	CLA	C3A-C2A-CAA-CBA
31	S1	604	CLA	CBA-CGA-O2A-C1
31	S1	604	CLA	O1A-CGA-O2A-C1
31	S1	604	CLA	CBD-CGD-O2D-CED
31	S1	605	CLA	C1A-C2A-CAA-CBA
31	S1	605	CLA	CHA-CBD-CGD-O1D
31	S1	605	CLA	CHA-CBD-CGD-O2D
31	S1	605	CLA	CBD-CGD-O2D-CED
31	S1	609	CLA	C1A-C2A-CAA-CBA
31	S1	609	CLA	CBD-CGD-O2D-CED
31	S1	610	CLA	C1A-C2A-CAA-CBA
31	S1	610	CLA	C3A-C2A-CAA-CBA
31	S1	610	CLA	CBD-CGD-O2D-CED
31	S1	611	CLA	C1A-C2A-CAA-CBA
31	S1	611	CLA	C3A-C2A-CAA-CBA
31	S1	613	CLA	CBD-CGD-O2D-CED
31	S1	617	CLA	CBD-CGD-O2D-CED
31	Y1	602	CLA	C11-C10-C8-C9
31	Y1	603	CLA	C6-C7-C8-C9
31	Y1	608	CLA	CHA-CBD-CGD-O1D
31	Y1	608	CLA	CHA-CBD-CGD-O2D
31	Y1	608	CLA	CBD-CGD-O2D-CED
31	Y1	611	CLA	CHA-CBD-CGD-O1D
31	Y1	611	CLA	CHA-CBD-CGD-O2D
31	Y1	611	CLA	CBD-CGD-O2D-CED
31	Y1	613	CLA	CHA-CBD-CGD-O1D
31	Y1	613	CLA	CHA-CBD-CGD-O2D
31	Y1	613	CLA	CBD-CGD-O2D-CED
31	a1	405	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	a1	405	CLA	CBD-CGD-O2D-CED
31	a1	406	CLA	C1A-C2A-CAA-CBA
31	a1	406	CLA	C3A-C2A-CAA-CBA
31	a1	406	CLA	CHA-CBD-CGD-O1D
31	a1	406	CLA	CHA-CBD-CGD-O2D
31	b1	602	CLA	CHA-CBD-CGD-O1D
31	b1	602	CLA	CHA-CBD-CGD-O2D
31	b1	603	CLA	C1A-C2A-CAA-CBA
31	b1	603	CLA	CHA-CBD-CGD-O1D
31	b1	603	CLA	CHA-CBD-CGD-O2D
31	b1	605	CLA	CHA-CBD-CGD-O1D
31	b1	605	CLA	CHA-CBD-CGD-O2D
31	b1	607	CLA	CBD-CGD-O2D-CED
31	b1	608	CLA	C1A-C2A-CAA-CBA
31	b1	608	CLA	C3A-C2A-CAA-CBA
31	b1	608	CLA	C2-C1-O2A-CGA
31	b1	608	CLA	CAD-CBD-CGD-O1D
31	b1	608	CLA	CAD-CBD-CGD-O2D
31	b1	608	CLA	CBD-CGD-O2D-CED
31	b1	608	CLA	C2-C3-C5-C6
31	b1	608	CLA	C4-C3-C5-C6
31	b1	609	CLA	C1A-C2A-CAA-CBA
31	b1	609	CLA	C3A-C2A-CAA-CBA
31	b1	609	CLA	CHA-CBD-CGD-O1D
31	b1	609	CLA	CHA-CBD-CGD-O2D
31	b1	610	CLA	C3A-C2A-CAA-CBA
31	b1	610	CLA	CHA-CBD-CGD-O1D
31	b1	610	CLA	CAD-CBD-CGD-O1D
31	b1	610	CLA	CAD-CBD-CGD-O2D
31	b1	611	CLA	CBD-CGD-O2D-CED
31	b1	612	CLA	CHA-CBD-CGD-O1D
31	b1	612	CLA	CHA-CBD-CGD-O2D
31	b1	612	CLA	CBD-CGD-O2D-CED
31	b1	613	CLA	C2-C1-O2A-CGA
31	b1	613	CLA	CHA-CBD-CGD-O1D
31	b1	613	CLA	CHA-CBD-CGD-O2D
31	b1	613	CLA	CAD-CBD-CGD-O1D
31	b1	614	CLA	C2-C1-O2A-CGA
31	b1	614	CLA	CBD-CGD-O2D-CED
31	b1	615	CLA	C1A-C2A-CAA-CBA
31	b1	615	CLA	C3A-C2A-CAA-CBA
31	b1	615	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b1	615	CLA	CHA-CBD-CGD-O2D
31	b1	616	CLA	CHA-CBD-CGD-O1D
31	b1	616	CLA	CHA-CBD-CGD-O2D
31	b1	616	CLA	CBD-CGD-O2D-CED
31	b1	617	CLA	C2-C1-O2A-CGA
31	b1	617	CLA	CBD-CGD-O2D-CED
31	c1	501	CLA	C1A-C2A-CAA-CBA
31	c1	501	CLA	CHA-CBD-CGD-O1D
31	c1	501	CLA	CHA-CBD-CGD-O2D
31	c1	501	CLA	CAD-CBD-CGD-O1D
31	c1	501	CLA	C4-C3-C5-C6
31	c1	502	CLA	CHA-CBD-CGD-O1D
31	c1	502	CLA	CHA-CBD-CGD-O2D
31	c1	502	CLA	CAD-CBD-CGD-O1D
31	c1	502	CLA	CAD-CBD-CGD-O2D
31	c1	503	CLA	C2-C3-C5-C6
31	c1	503	CLA	C4-C3-C5-C6
31	c1	504	CLA	CAD-CBD-CGD-O1D
31	c1	504	CLA	CBD-CGD-O2D-CED
31	c1	505	CLA	C1A-C2A-CAA-CBA
31	c1	506	CLA	C2-C1-O2A-CGA
31	c1	506	CLA	CHA-CBD-CGD-O1D
31	c1	506	CLA	CHA-CBD-CGD-O2D
31	c1	506	CLA	CAD-CBD-CGD-O1D
31	c1	508	CLA	CHA-CBD-CGD-O1D
31	c1	508	CLA	CHA-CBD-CGD-O2D
31	c1	509	CLA	C6-C7-C8-C9
31	c1	511	CLA	C1A-C2A-CAA-CBA
31	c1	512	CLA	CBA-CGA-O2A-C1
31	c1	512	CLA	O1A-CGA-O2A-C1
31	c1	512	CLA	CBD-CGD-O2D-CED
31	c1	513	CLA	C1A-C2A-CAA-CBA
31	c1	513	CLA	CBD-CGD-O2D-CED
31	d1	402	CLA	CHA-CBD-CGD-O1D
31	d1	402	CLA	CHA-CBD-CGD-O2D
31	d1	402	CLA	C2-C3-C5-C6
31	d1	402	CLA	C4-C3-C5-C6
31	d1	403	CLA	CBA-CGA-O2A-C1
31	d1	403	CLA	CBD-CGD-O2D-CED
31	d1	403	CLA	C2-C3-C5-C6
31	d1	403	CLA	C4-C3-C5-C6
31	n1	604	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	n1	604	CLA	C3A-C2A-CAA-CBA
31	n1	604	CLA	CHA-CBD-CGD-O1D
31	n1	610	CLA	C1A-C2A-CAA-CBA
31	n1	613	CLA	C1A-C2A-CAA-CBA
31	n1	614	CLA	C1A-C2A-CAA-CBA
31	g1	602	CLA	C1A-C2A-CAA-CBA
31	g1	602	CLA	C3A-C2A-CAA-CBA
31	g1	603	CLA	C3A-C2A-CAA-CBA
31	g1	604	CLA	C2-C1-O2A-CGA
31	g1	604	CLA	CBD-CGD-O2D-CED
31	g1	610	CLA	CHA-CBD-CGD-O1D
31	g1	610	CLA	CBD-CGD-O2D-CED
31	g1	611	CLA	CHA-CBD-CGD-O1D
31	g1	611	CLA	CBD-CGD-O2D-CED
31	g1	613	CLA	CHA-CBD-CGD-O1D
31	g1	613	CLA	CHA-CBD-CGD-O2D
31	g1	614	CLA	CBA-CGA-O2A-C1
31	g1	614	CLA	O1A-CGA-O2A-C1
31	r1	603	CLA	C1A-C2A-CAA-CBA
31	r1	603	CLA	C3A-C2A-CAA-CBA
31	r1	603	CLA	CHA-CBD-CGD-O1D
31	r1	603	CLA	CHA-CBD-CGD-O2D
31	r1	603	CLA	CBD-CGD-O2D-CED
31	r1	604	CLA	CHA-CBD-CGD-O1D
31	r1	604	CLA	CHA-CBD-CGD-O2D
31	r1	608	CLA	C1A-C2A-CAA-CBA
31	r1	608	CLA	C3A-C2A-CAA-CBA
31	r1	608	CLA	CBD-CGD-O2D-CED
31	r1	608	CLA	C2-C3-C5-C6
31	r1	608	CLA	C4-C3-C5-C6
31	r1	609	CLA	CBD-CGD-O2D-CED
31	r1	610	CLA	CHA-CBD-CGD-O1D
31	r1	610	CLA	CHA-CBD-CGD-O2D
31	r1	612	CLA	C1A-C2A-CAA-CBA
31	r1	612	CLA	C3A-C2A-CAA-CBA
31	r1	612	CLA	CBD-CGD-O2D-CED
31	s1	602	CLA	C2-C1-O2A-CGA
31	s1	602	CLA	CHA-CBD-CGD-O2D
31	s1	603	CLA	C3A-C2A-CAA-CBA
31	s1	603	CLA	CHA-CBD-CGD-O1D
31	s1	603	CLA	CHA-CBD-CGD-O2D
31	s1	605	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s1	605	CLA	CBA-CGA-O2A-C1
31	s1	605	CLA	CHA-CBD-CGD-O1D
31	s1	609	CLA	C3A-C2A-CAA-CBA
31	s1	610	CLA	C1A-C2A-CAA-CBA
31	s1	610	CLA	C3A-C2A-CAA-CBA
31	s1	611	CLA	C1A-C2A-CAA-CBA
31	s1	611	CLA	C3A-C2A-CAA-CBA
31	s1	611	CLA	CBD-CGD-O2D-CED
31	s1	613	CLA	CHA-CBD-CGD-O1D
31	s1	613	CLA	CHA-CBD-CGD-O2D
31	s1	613	CLA	CBD-CGD-O2D-CED
31	s1	614	CLA	C2A-CAA-CBA-CGA
31	s1	617	CLA	C2A-CAA-CBA-CGA
31	s1	617	CLA	C2-C1-O2A-CGA
31	y1	602	CLA	CBD-CGD-O2D-CED
31	y1	608	CLA	CHA-CBD-CGD-O1D
31	y1	608	CLA	CHA-CBD-CGD-O2D
31	y1	610	CLA	CHA-CBD-CGD-O1D
31	y1	610	CLA	CHA-CBD-CGD-O2D
31	y1	610	CLA	CBD-CGD-O2D-CED
31	y1	612	CLA	CHA-CBD-CGD-O1D
31	y1	612	CLA	CHA-CBD-CGD-O2D
31	y1	613	CLA	CBD-CGD-O2D-CED
32	A	409	PHO	C3A-C2A-CAA-CBA
32	a	408	PHO	C2A-CAA-CBA-CGA
32	A1	409	PHO	C1A-C2A-CAA-CBA
32	A1	409	PHO	C3A-C2A-CAA-CBA
32	a1	409	PHO	CBD-CGD-O2D-CED
33	A	411	BCR	C11-C10-C9-C8
33	A	411	BCR	C11-C10-C9-C34
33	A	411	BCR	C10-C11-C12-C13
33	A	411	BCR	C11-C12-C13-C14
33	A	411	BCR	C11-C12-C13-C35
33	A	411	BCR	C17-C18-C19-C20
33	A	411	BCR	C36-C18-C19-C20
33	A	411	BCR	C23-C24-C25-C30
33	B	618	BCR	C11-C10-C9-C8
33	B	618	BCR	C11-C10-C9-C34
33	B	618	BCR	C10-C11-C12-C13
33	B	618	BCR	C17-C18-C19-C20
33	B	618	BCR	C36-C18-C19-C20
33	B	618	BCR	C21-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	B	618	BCR	C37-C22-C23-C24
33	C	514	BCR	C11-C10-C9-C8
33	C	514	BCR	C11-C10-C9-C34
33	C	514	BCR	C9-C10-C11-C12
33	C	514	BCR	C10-C11-C12-C13
33	C	515	BCR	C7-C8-C9-C10
33	C	515	BCR	C7-C8-C9-C34
33	C	515	BCR	C11-C10-C9-C34
33	C	515	BCR	C17-C18-C19-C20
33	C	515	BCR	C36-C18-C19-C20
33	C	516	BCR	C1-C6-C7-C8
33	C	516	BCR	C5-C6-C7-C8
33	C	516	BCR	C7-C8-C9-C10
33	C	516	BCR	C7-C8-C9-C34
33	C	516	BCR	C11-C10-C9-C8
33	C	516	BCR	C11-C10-C9-C34
33	C	516	BCR	C10-C11-C12-C13
33	C	516	BCR	C17-C18-C19-C20
33	C	516	BCR	C36-C18-C19-C20
33	C	517	BCR	C11-C10-C9-C8
33	C	517	BCR	C11-C10-C9-C34
33	C	517	BCR	C10-C11-C12-C13
33	C	517	BCR	C17-C18-C19-C20
33	C	517	BCR	C36-C18-C19-C20
33	D	404	BCR	C11-C10-C9-C8
33	D	404	BCR	C11-C10-C9-C34
33	D	404	BCR	C10-C11-C12-C13
33	D	404	BCR	C23-C24-C25-C30
33	a	411	BCR	C11-C10-C9-C8
33	a	411	BCR	C11-C10-C9-C34
33	a	411	BCR	C10-C11-C12-C13
33	a	411	BCR	C17-C18-C19-C20
33	a	411	BCR	C36-C18-C19-C20
33	a	411	BCR	C23-C24-C25-C30
33	b	618	BCR	C7-C8-C9-C34
33	b	618	BCR	C11-C10-C9-C8
33	b	618	BCR	C11-C10-C9-C34
33	b	618	BCR	C10-C11-C12-C13
33	b	618	BCR	C36-C18-C19-C20
33	b	619	BCR	C11-C10-C9-C8
33	b	619	BCR	C11-C10-C9-C34
33	b	619	BCR	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
33	b	619	BCR	C21-C22-C23-C24
33	b	619	BCR	C37-C22-C23-C24
33	c	514	BCR	C10-C11-C12-C13
33	c	514	BCR	C23-C24-C25-C30
33	c	515	BCR	C11-C10-C9-C8
33	c	515	BCR	C11-C10-C9-C34
33	c	515	BCR	C10-C11-C12-C13
33	c	515	BCR	C17-C18-C19-C20
33	c	515	BCR	C36-C18-C19-C20
33	c	516	BCR	C1-C6-C7-C8
33	c	516	BCR	C7-C8-C9-C10
33	c	516	BCR	C7-C8-C9-C34
33	c	516	BCR	C11-C10-C9-C8
33	c	516	BCR	C11-C10-C9-C34
33	c	516	BCR	C10-C11-C12-C13
33	c	516	BCR	C21-C22-C23-C24
33	c	516	BCR	C37-C22-C23-C24
33	c	517	BCR	C11-C10-C9-C8
33	c	517	BCR	C11-C10-C9-C34
33	c	517	BCR	C10-C11-C12-C13
33	c	517	BCR	C36-C18-C19-C20
33	d	404	BCR	C11-C10-C9-C8
33	d	404	BCR	C11-C10-C9-C34
33	d	404	BCR	C10-C11-C12-C13
33	A1	411	BCR	C11-C10-C9-C8
33	A1	411	BCR	C11-C10-C9-C34
33	A1	411	BCR	C17-C18-C19-C20
33	A1	411	BCR	C36-C18-C19-C20
33	B1	618	BCR	C11-C10-C9-C8
33	B1	618	BCR	C11-C10-C9-C34
33	B1	618	BCR	C9-C10-C11-C12
33	B1	618	BCR	C10-C11-C12-C13
33	B1	618	BCR	C17-C18-C19-C20
33	B1	618	BCR	C36-C18-C19-C20
33	B1	619	BCR	C7-C8-C9-C10
33	B1	619	BCR	C7-C8-C9-C34
33	B1	619	BCR	C11-C10-C9-C8
33	B1	619	BCR	C11-C10-C9-C34
33	C1	514	BCR	C11-C10-C9-C8
33	C1	514	BCR	C11-C10-C9-C34
33	C1	514	BCR	C9-C10-C11-C12
33	C1	514	BCR	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
33	C1	515	BCR	C11-C10-C9-C8
33	C1	515	BCR	C11-C10-C9-C34
33	C1	515	BCR	C10-C11-C12-C13
33	C1	516	BCR	C1-C6-C7-C8
33	C1	516	BCR	C5-C6-C7-C8
33	C1	516	BCR	C7-C8-C9-C10
33	C1	516	BCR	C7-C8-C9-C34
33	C1	516	BCR	C11-C10-C9-C8
33	C1	516	BCR	C11-C10-C9-C34
33	C1	516	BCR	C10-C11-C12-C13
33	C1	516	BCR	C11-C12-C13-C14
33	C1	516	BCR	C11-C12-C13-C35
33	C1	516	BCR	C17-C18-C19-C20
33	C1	516	BCR	C36-C18-C19-C20
33	C1	516	BCR	C21-C22-C23-C24
33	C1	517	BCR	C11-C10-C9-C8
33	C1	517	BCR	C11-C10-C9-C34
33	C1	517	BCR	C17-C18-C19-C20
33	C1	517	BCR	C36-C18-C19-C20
33	C1	517	BCR	C23-C24-C25-C26
33	D1	404	BCR	C11-C10-C9-C8
33	D1	404	BCR	C11-C10-C9-C34
33	D1	404	BCR	C21-C22-C23-C24
33	D1	404	BCR	C37-C22-C23-C24
33	D1	404	BCR	C23-C24-C25-C26
33	D1	404	BCR	C23-C24-C25-C30
33	a1	411	BCR	C11-C10-C9-C8
33	a1	411	BCR	C11-C10-C9-C34
33	a1	411	BCR	C10-C11-C12-C13
33	a1	411	BCR	C17-C18-C19-C20
33	a1	411	BCR	C36-C18-C19-C20
33	a1	411	BCR	C21-C22-C23-C24
33	a1	411	BCR	C37-C22-C23-C24
33	b1	618	BCR	C11-C10-C9-C8
33	b1	618	BCR	C11-C10-C9-C34
33	b1	618	BCR	C10-C11-C12-C13
33	b1	618	BCR	C17-C18-C19-C20
33	b1	618	BCR	C36-C18-C19-C20
33	b1	619	BCR	C11-C10-C9-C8
33	b1	619	BCR	C11-C10-C9-C34
33	b1	619	BCR	C10-C11-C12-C13
33	c1	514	BCR	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	c1	514	BCR	C11-C10-C9-C34
33	c1	514	BCR	C10-C11-C12-C13
33	c1	514	BCR	C17-C18-C19-C20
33	c1	514	BCR	C36-C18-C19-C20
33	c1	514	BCR	C23-C24-C25-C30
33	c1	515	BCR	C11-C10-C9-C8
33	c1	515	BCR	C11-C10-C9-C34
33	c1	515	BCR	C11-C12-C13-C14
33	c1	515	BCR	C17-C18-C19-C20
33	c1	515	BCR	C36-C18-C19-C20
33	c1	515	BCR	C23-C24-C25-C30
33	c1	516	BCR	C11-C10-C9-C8
33	c1	516	BCR	C11-C10-C9-C34
33	c1	516	BCR	C17-C18-C19-C20
33	c1	516	BCR	C36-C18-C19-C20
33	c1	516	BCR	C21-C22-C23-C24
33	c1	516	BCR	C37-C22-C23-C24
33	c1	517	BCR	C11-C10-C9-C8
33	c1	517	BCR	C11-C10-C9-C34
33	c1	517	BCR	C17-C18-C19-C20
33	c1	517	BCR	C36-C18-C19-C20
33	d1	404	BCR	C11-C10-C9-C8
33	d1	404	BCR	C11-C10-C9-C34
33	d1	404	BCR	C11-C12-C13-C14
33	d1	404	BCR	C11-C12-C13-C35
33	d1	404	BCR	C21-C22-C23-C24
33	d1	404	BCR	C37-C22-C23-C24
33	d1	404	BCR	C23-C24-C25-C26
33	d1	404	BCR	C23-C24-C25-C30
34	A	412	SQD	C2-C1-O6-C44
34	A	412	SQD	O5-C1-O6-C44
34	A	412	SQD	O5-C5-C6-S
34	B	621	SQD	O49-C7-O47-C45
34	B	621	SQD	C8-C7-O47-C45
34	B	621	SQD	O5-C5-C6-S
34	C	526	SQD	O5-C5-C6-S
34	C	526	SQD	C5-C6-S-O7
34	C	526	SQD	C5-C6-S-O8
34	C	526	SQD	C5-C6-S-O9
34	a	412	SQD	O5-C1-O6-C44
34	a	412	SQD	O5-C5-C6-S
34	b	621	SQD	O49-C7-O47-C45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	b	621	SQD	C8-C7-O47-C45
34	c	626	SQD	O5-C5-C6-S
34	c	626	SQD	C5-C6-S-O7
34	c	626	SQD	C5-C6-S-O8
34	c	626	SQD	C5-C6-S-O9
34	A1	412	SQD	C45-C44-O6-C1
34	B1	621	SQD	O5-C1-O6-C44
34	B1	626	SQD	C2-C1-O6-C44
34	B1	626	SQD	O5-C1-O6-C44
34	B1	626	SQD	C5-C6-S-O7
34	B1	626	SQD	C5-C6-S-O8
34	B1	626	SQD	C5-C6-S-O9
34	C1	526	SQD	C5-C6-S-O9
34	a1	412	SQD	O5-C5-C6-S
34	b1	621	SQD	C2-C1-O6-C44
34	b1	621	SQD	O5-C1-O6-C44
34	b1	621	SQD	O5-C5-C6-S
34	b1	626	SQD	C2-C1-O6-C44
34	b1	626	SQD	O5-C1-O6-C44
34	b1	626	SQD	C5-C6-S-O7
34	b1	626	SQD	C5-C6-S-O8
34	b1	626	SQD	C5-C6-S-O9
34	m1	101	SQD	O5-C5-C6-S
34	m1	101	SQD	C5-C6-S-O7
34	m1	101	SQD	C5-C6-S-O8
34	m1	101	SQD	C5-C6-S-O9
35	A	413	LMG	C11-C10-O7-C8
35	C	521	LMG	C2-C1-O1-C7
35	C	521	LMG	O6-C1-O1-C7
35	C	521	LMG	C11-C10-O7-C8
35	J	101	LMG	O6-C1-O1-C7
35	J	101	LMG	O7-C8-C9-O8
35	a	413	LMG	O6-C1-O1-C7
35	b	622	LMG	O9-C10-O7-C8
35	c	521	LMG	C2-C1-O1-C7
35	c	521	LMG	O6-C1-O1-C7
35	c	521	LMG	O9-C10-O7-C8
35	j	101	LMG	O7-C8-C9-O8
35	A1	413	LMG	O6-C1-O1-C7
35	B1	622	LMG	C2-C1-O1-C7
35	B1	622	LMG	O6-C1-O1-C7
35	B1	622	LMG	O9-C10-O7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	W1	201	LMG	C11-C10-O7-C8
35	a1	413	LMG	O6-C1-O1-C7
35	b1	622	LMG	O6-C1-O1-C7
35	b1	622	LMG	O9-C10-O7-C8
35	b1	622	LMG	C11-C10-O7-C8
37	B	620	C7Z	C1-C6-C7-C8
37	B	620	C7Z	C7-C8-C9-C19
37	B	620	C7Z	C7-C8-C9-C10
37	b	620	C7Z	C9-C10-C11-C12
37	b	620	C7Z	C11-C12-C13-C20
37	b	620	C7Z	C11-C12-C13-C14
37	B1	620	C7Z	C5-C6-C7-C8
37	b1	620	C7Z	C5-C6-C7-C8
37	b1	620	C7Z	C21-C26-C27-C28
37	b1	620	C7Z	C11-C12-C13-C20
37	b1	620	C7Z	C11-C12-C13-C14
37	b1	620	C7Z	C31-C32-C33-C34
37	b1	620	C7Z	C31-C32-C33-C40
37	b1	620	C7Z	C27-C28-C29-C30
37	b1	620	C7Z	C27-C28-C29-C39
38	B	625	DGA	CG1-CG2-CG3-OXT
38	B	625	DGA	OG2-CG2-CG3-OXT
38	C	524	DGA	CG1-CG2-CG3-OXT
38	C	524	DGA	OG2-CG2-CG3-OXT
38	b	623	DGA	CB2-CB1-OG2-CG2
38	b	623	DGA	CG1-CG2-CG3-OXT
38	b	623	DGA	OG2-CG2-CG3-OXT
38	c	524	DGA	OG2-CG2-CG3-OXT
38	C1	524	DGA	CG1-CG2-CG3-OXT
38	C1	524	DGA	OG2-CG2-CG3-OXT
39	b	625	GOL	O1-C1-C2-O2
39	b	625	GOL	O1-C1-C2-C3
40	C	519	DGD	C2E-C1E-O5D-C6D
40	C	519	DGD	O6E-C1E-O5D-C6D
40	C	520	DGD	C2B-C1B-O2G-C2G
40	C	523	DGD	C2A-C1A-O1G-C1G
40	C	523	DGD	O1A-C1A-O1G-C1G
40	C	523	DGD	O1B-C1B-O2G-C2G
40	C	523	DGD	C2E-C1E-O5D-C6D
40	C	523	DGD	O6E-C1E-O5D-C6D
40	c	519	DGD	C2E-C1E-O5D-C6D
40	c	519	DGD	O6E-C1E-O5D-C6D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
40	c	520	DGD	C2B-C1B-O2G-C2G
40	c	523	DGD	C2A-C1A-O1G-C1G
40	c	523	DGD	O1A-C1A-O1G-C1G
40	c	523	DGD	C2B-C1B-O2G-C2G
40	c	523	DGD	O1B-C1B-O2G-C2G
40	c	523	DGD	C2E-C1E-O5D-C6D
40	c	523	DGD	O6E-C1E-O5D-C6D
40	B1	623	DGD	C2B-C1B-O2G-C2G
40	B1	623	DGD	O6D-C1D-O3G-C3G
40	B1	623	DGD	C2E-C1E-O5D-C6D
40	B1	623	DGD	O6E-C1E-O5D-C6D
40	b1	623	DGD	C2B-C1B-O2G-C2G
40	b1	623	DGD	O1B-C1B-O2G-C2G
40	b1	623	DGD	O6D-C1D-O3G-C3G
40	b1	623	DGD	C2E-C1E-O5D-C6D
40	b1	623	DGD	O6E-C1E-O5D-C6D
41	C	525	LHG	C1-C2-C3-O3
41	C	525	LHG	C3-O3-P-O4
41	D	408	LHG	C1-C2-C3-O3
41	D	408	LHG	C3-O3-P-O4
41	D	408	LHG	C3-O3-P-O5
41	D	408	LHG	C3-O3-P-O6
41	D	409	LHG	C1-C2-C3-O3
41	D	410	LHG	C3-O3-P-O4
41	D	410	LHG	C3-O3-P-O5
41	D	410	LHG	C3-O3-P-O6
41	D	410	LHG	C4-O6-P-O3
41	D	410	LHG	O6-C4-C5-O7
41	L	101	LHG	C3-O3-P-O4
41	L	101	LHG	C3-O3-P-O5
41	L	101	LHG	C3-O3-P-O6
41	L	101	LHG	C4-O6-P-O5
41	N	624	LHG	C1-C2-C3-O3
41	N	624	LHG	O2-C2-C3-O3
41	N	624	LHG	O9-C7-O7-C5
41	G	630	LHG	O1-C1-C2-C3
41	G	630	LHG	C4-O6-P-O4
41	G	630	LHG	O7-C5-C6-O8
41	G	630	LHG	C8-C7-O7-C5
41	S	624	LHG	C3-O3-P-O6
41	S	624	LHG	O6-C4-C5-O7
41	S	624	LHG	C8-C7-O7-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	Y	624	LHG	C1-C2-C3-O3
41	Y	624	LHG	O2-C2-C3-O3
41	Y	624	LHG	C4-O6-P-O3
41	Y	624	LHG	C4-O6-P-O4
41	Y	624	LHG	C4-O6-P-O5
41	Y	624	LHG	O7-C5-C6-O8
41	c	625	LHG	O1-C1-C2-C3
41	c	625	LHG	O2-C2-C3-O3
41	c	625	LHG	C3-O3-P-O5
41	c	625	LHG	C3-O3-P-O6
41	c	625	LHG	C4-O6-P-O3
41	c	625	LHG	C4-O6-P-O4
41	c	625	LHG	C4-O6-P-O5
41	d	408	LHG	O1-C1-C2-C3
41	d	408	LHG	C4-O6-P-O3
41	d	408	LHG	C8-C7-O7-C5
41	d	409	LHG	C1-C2-C3-O3
41	d	410	LHG	C3-O3-P-O4
41	d	410	LHG	C3-O3-P-O5
41	d	410	LHG	C4-O6-P-O5
41	l	101	LHG	C4-O6-P-O3
41	l	101	LHG	C4-O6-P-O5
41	n	624	LHG	O1-C1-C2-O2
41	n	624	LHG	C4-O6-P-O3
41	n	624	LHG	O9-C7-O7-C5
41	g	624	LHG	O1-C1-C2-C3
41	g	624	LHG	C1-C2-C3-O3
41	g	624	LHG	C4-O6-P-O4
41	s	624	LHG	C1-C2-C3-O3
41	s	624	LHG	O2-C2-C3-O3
41	s	624	LHG	C8-C7-O7-C5
41	y	624	LHG	O1-C1-C2-C3
41	y	624	LHG	C4-O6-P-O5
41	C1	525	LHG	C1-C2-C3-O3
41	C1	525	LHG	C3-O3-P-O6
41	C1	525	LHG	C4-O6-P-O4
41	D1	408	LHG	O1-C1-C2-C3
41	D1	408	LHG	C4-O6-P-O5
41	D1	409	LHG	C1-C2-C3-O3
41	D1	410	LHG	O1-C1-C2-O2
41	D1	410	LHG	O1-C1-C2-C3
41	D1	410	LHG	C3-O3-P-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	D1	410	LHG	C3-O3-P-O5
41	D1	410	LHG	C3-O3-P-O6
41	D1	410	LHG	C4-O6-P-O3
41	D1	410	LHG	C4-O6-P-O4
41	D1	410	LHG	C4-O6-P-O5
41	D1	410	LHG	O7-C5-C6-O8
41	L1	101	LHG	O1-C1-C2-C3
41	L1	101	LHG	C3-O3-P-O4
41	L1	101	LHG	O9-C7-O7-C5
41	L1	101	LHG	C8-C7-O7-C5
41	N1	624	LHG	O1-C1-C2-C3
41	N1	624	LHG	C1-C2-C3-O3
41	N1	624	LHG	O2-C2-C3-O3
41	N1	624	LHG	C4-O6-P-O5
41	N1	624	LHG	O7-C5-C6-O8
41	G1	624	LHG	C4-O6-P-O4
41	G1	624	LHG	O7-C5-C6-O8
41	S1	624	LHG	O1-C1-C2-C3
41	S1	624	LHG	C3-O3-P-O5
41	S1	624	LHG	C4-O6-P-O4
41	S1	624	LHG	C4-O6-P-O5
41	Y1	624	LHG	C4-O6-P-O4
41	Y1	624	LHG	C4-O6-P-O5
41	c1	525	LHG	C4-O6-P-O4
41	d1	408	LHG	O1-C1-C2-C3
41	d1	408	LHG	C3-O3-P-O5
41	d1	408	LHG	C3-O3-P-O6
41	d1	409	LHG	O1-C1-C2-C3
41	d1	409	LHG	C1-C2-C3-O3
41	d1	409	LHG	C3-O3-P-O5
41	d1	409	LHG	C3-O3-P-O6
41	d1	409	LHG	C4-O6-P-O3
41	d1	410	LHG	C3-O3-P-O5
41	d1	410	LHG	C4-O6-P-O4
41	d1	410	LHG	C4-O6-P-O5
41	d1	410	LHG	O7-C5-C6-O8
41	n1	624	LHG	C4-O6-P-O4
41	n1	624	LHG	O7-C5-C6-O8
41	n1	624	LHG	C8-C7-O7-C5
41	g1	624	LHG	C4-O6-P-O4
41	g1	624	LHG	O7-C5-C6-O8
41	g1	624	LHG	O9-C7-O7-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	g1	624	LHG	C8-C7-O7-C5
41	s1	624	LHG	O1-C1-C2-C3
41	s1	624	LHG	C3-O3-P-O5
41	s1	624	LHG	C4-O6-P-O3
41	s1	624	LHG	C4-O6-P-O5
41	y1	624	LHG	O1-C1-C2-C3
41	y1	624	LHG	C1-C2-C3-O3
41	y1	624	LHG	O2-C2-C3-O3
41	y1	624	LHG	C3-O3-P-O5
41	y1	624	LHG	C4-O6-P-O5
42	C	527	LMK	O9-C10-C11-C12
42	C	527	LMK	O9-C10-O7-C8
42	C	527	LMK	O10-C28-O8-C9
42	c	627	LMK	O9-C10-O7-C8
42	c	627	LMK	O10-C28-C29-C30
42	C1	527	LMK	O9-C10-O7-C8
42	C1	527	LMK	C1-C2-C3-C4
42	C1	527	LMK	C1-C2-C3-N4
42	C1	527	LMK	C2-C3-N4-C5
42	C1	527	LMK	C2-C3-N4-C6
42	C1	527	LMK	C2-C3-N4-C46
42	C1	527	LMK	O10-C28-O8-C9
42	c1	527	LMK	O1-C7-C8-O7
42	c1	527	LMK	O10-C28-C29-C30
44	D	405	PL9	C7-C8-C9-C11
44	D	405	PL9	C12-C11-C9-C8
44	D	405	PL9	C12-C13-C14-C15
44	D	405	PL9	C37-C38-C39-C41
44	D	405	PL9	C42-C43-C44-C45
44	d	405	PL9	C12-C13-C14-C16
44	D1	405	PL9	C20-C19-C21-C22
44	D1	405	PL9	C22-C23-C24-C25
44	D1	405	PL9	C37-C38-C39-C40
44	d1	405	PL9	C20-C19-C21-C22
44	d1	405	PL9	C22-C23-C24-C26
44	d1	405	PL9	C32-C33-C34-C35
44	d1	405	PL9	C32-C33-C34-C36
44	d1	405	PL9	C35-C34-C36-C37
44	d1	405	PL9	C37-C38-C39-C40
46	H	101	RRX	C37-C22-C23-C24
46	H	101	RRX	C21-C22-C23-C24
46	H	101	RRX	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
46	H	101	RRX	C7-C8-C9-C34
46	h	101	RRX	C7-C8-C9-C10
46	h	101	RRX	C7-C8-C9-C34
46	H1	101	RRX	C23-C24-C25-C26
46	h1	101	RRX	C23-C24-C25-C26
46	h1	101	RRX	C36-C18-C19-C20
46	h1	101	RRX	C17-C18-C19-C20
46	h1	101	RRX	C13-C14-C15-C16
46	h1	101	RRX	C5-C6-C7-C8
47	N	601	CHL	C2-C3-C5-C6
47	N	601	CHL	C4-C3-C5-C6
47	G	601	CHL	CHA-CBD-CGD-O1D
47	G	601	CHL	CHA-CBD-CGD-O2D
47	G	601	CHL	C4-C3-C5-C6
47	G	606	CHL	C1A-C2A-CAA-CBA
47	G	606	CHL	C3A-C2A-CAA-CBA
47	G	607	CHL	C1A-C2A-CAA-CBA
47	R	606	CHL	CHA-CBD-CGD-O1D
47	R	606	CHL	CHA-CBD-CGD-O2D
47	R	606	CHL	CAD-CBD-CGD-O1D
47	R	607	CHL	CHA-CBD-CGD-O1D
47	R	607	CHL	CHA-CBD-CGD-O2D
47	S	601	CHL	CHA-CBD-CGD-O1D
47	S	601	CHL	CHA-CBD-CGD-O2D
47	Y	601	CHL	CHA-CBD-CGD-O1D
47	Y	601	CHL	CHA-CBD-CGD-O2D
47	Y	601	CHL	C2-C3-C5-C6
47	Y	601	CHL	C4-C3-C5-C6
47	n	609	CHL	C1A-C2A-CAA-CBA
47	g	601	CHL	CHA-CBD-CGD-O1D
47	g	601	CHL	CHA-CBD-CGD-O2D
47	g	605	CHL	CHA-CBD-CGD-O1D
47	g	605	CHL	CHA-CBD-CGD-O2D
47	g	606	CHL	C1A-C2A-CAA-CBA
47	g	607	CHL	C1A-C2A-CAA-CBA
47	g	608	CHL	CHA-CBD-CGD-O1D
47	g	608	CHL	CHA-CBD-CGD-O2D
47	g	609	CHL	C2-C3-C5-C6
47	g	609	CHL	C4-C3-C5-C6
47	r	607	CHL	CHA-CBD-CGD-O1D
47	r	607	CHL	CHA-CBD-CGD-O2D
47	s	601	CHL	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	s	601	CHL	CHA-CBD-CGD-O2D
47	s	607	CHL	C1A-C2A-CAA-CBA
47	y	601	CHL	CHA-CBD-CGD-O1D
47	y	601	CHL	CHA-CBD-CGD-O2D
47	y	601	CHL	C4-C3-C5-C6
47	y	601	CHL	C11-C12-C13-C14
47	y	605	CHL	C1A-C2A-CAA-CBA
47	y	609	CHL	CHA-CBD-CGD-O1D
47	N1	606	CHL	C2-C3-C5-C6
47	N1	606	CHL	C4-C3-C5-C6
47	N1	607	CHL	C1A-C2A-CAA-CBA
47	N1	608	CHL	CHA-CBD-CGD-O1D
47	N1	608	CHL	CHA-CBD-CGD-O2D
47	N1	609	CHL	CHA-CBD-CGD-O1D
47	N1	609	CHL	CHA-CBD-CGD-O2D
47	N1	609	CHL	CAD-CBD-CGD-O1D
47	N1	609	CHL	CAD-CBD-CGD-O2D
47	G1	605	CHL	C1A-C2A-CAA-CBA
47	G1	605	CHL	C3A-C2A-CAA-CBA
47	G1	605	CHL	CHA-CBD-CGD-O1D
47	G1	605	CHL	CHA-CBD-CGD-O2D
47	G1	609	CHL	CHA-CBD-CGD-O1D
47	G1	609	CHL	CHA-CBD-CGD-O2D
47	R1	607	CHL	CHA-CBD-CGD-O1D
47	R1	607	CHL	CHA-CBD-CGD-O2D
47	S1	601	CHL	CHA-CBD-CGD-O1D
47	S1	601	CHL	CHA-CBD-CGD-O2D
47	Y1	601	CHL	CHA-CBD-CGD-O1D
47	Y1	601	CHL	CHA-CBD-CGD-O2D
47	Y1	609	CHL	CHA-CBD-CGD-O1D
47	Y1	609	CHL	CHA-CBD-CGD-O2D
47	n1	605	CHL	C2A-CAA-CBA-CGA
47	g1	601	CHL	C3A-C2A-CAA-CBA
47	g1	601	CHL	CHA-CBD-CGD-O1D
47	g1	601	CHL	CHA-CBD-CGD-O2D
47	g1	605	CHL	CHA-CBD-CGD-O1D
47	g1	605	CHL	CHA-CBD-CGD-O2D
47	g1	607	CHL	C1A-C2A-CAA-CBA
47	g1	609	CHL	C4-C3-C5-C6
47	r1	607	CHL	CHA-CBD-CGD-O1D
47	r1	607	CHL	CHA-CBD-CGD-O2D
47	s1	606	CHL	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	y1	601	CHL	CHA-CBD-CGD-O1D
47	y1	601	CHL	CHA-CBD-CGD-O2D
47	y1	607	CHL	CHA-CBD-CGD-O1D
48	N	620	LUT	C25-C26-C27-C28
48	N	620	LUT	C27-C28-C29-C30
48	N	620	LUT	C27-C28-C29-C39
48	G	620	LUT	C27-C28-C29-C30
48	G	620	LUT	C27-C28-C29-C39
48	G	621	LUT	C31-C32-C33-C34
48	G	621	LUT	C31-C32-C33-C40
48	R	620	LUT	C31-C32-C33-C34
48	R	620	LUT	C31-C32-C33-C40
48	S	620	LUT	C21-C26-C27-C28
48	S	620	LUT	C25-C26-C27-C28
48	Y	620	LUT	C27-C28-C29-C30
48	Y	620	LUT	C27-C28-C29-C39
48	Y	621	LUT	C21-C26-C27-C28
48	n	620	LUT	C25-C26-C27-C28
48	n	620	LUT	C31-C32-C33-C34
48	n	620	LUT	C31-C32-C33-C40
48	n	621	LUT	C21-C26-C27-C28
48	g	620	LUT	C31-C32-C33-C34
48	g	620	LUT	C31-C32-C33-C40
48	r	620	LUT	C31-C32-C33-C34
48	r	620	LUT	C31-C32-C33-C40
48	r	620	LUT	C33-C34-C35-C15
48	s	620	LUT	C21-C26-C27-C28
48	s	621	LUT	C25-C26-C27-C28
48	y	621	LUT	C31-C32-C33-C40
48	N1	620	LUT	C1-C6-C7-C8
48	N1	620	LUT	C27-C28-C29-C30
48	N1	620	LUT	C27-C28-C29-C39
48	N1	621	LUT	C21-C26-C27-C28
48	G1	621	LUT	C21-C26-C27-C28
48	R1	620	LUT	C27-C28-C29-C30
48	R1	620	LUT	C27-C28-C29-C39
48	S1	620	LUT	C25-C26-C27-C28
48	Y1	620	LUT	C27-C28-C29-C39
48	Y1	621	LUT	C21-C26-C27-C28
48	n1	620	LUT	C27-C28-C29-C39
48	n1	621	LUT	C21-C26-C27-C28
48	g1	620	LUT	C27-C28-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
48	g1	620	LUT	C27-C28-C29-C39
48	g1	621	LUT	C21-C26-C27-C28
48	r1	620	LUT	C7-C8-C9-C10
48	r1	620	LUT	C7-C8-C9-C19
48	r1	620	LUT	C31-C32-C33-C34
48	r1	620	LUT	C31-C32-C33-C40
48	s1	620	LUT	C21-C26-C27-C28
48	y1	620	LUT	C27-C28-C29-C30
48	y1	620	LUT	C27-C28-C29-C39
48	y1	621	LUT	C21-C26-C27-C28
49	R	621	XAT	C7-C8-C9-C19
49	R	621	XAT	C9-C10-C11-C12
49	R	621	XAT	C10-C11-C12-C13
49	R	621	XAT	C12-C13-C14-C15
49	R	621	XAT	C20-C13-C14-C15
49	Y	622	XAT	C26-C27-C28-C29
49	r	622	XAT	C7-C8-C9-C10
49	r	622	XAT	C7-C8-C9-C19
49	r	622	XAT	C10-C11-C12-C13
49	r	622	XAT	C26-C27-C28-C29
49	Y1	622	XAT	C27-C28-C29-C39
49	n1	622	XAT	C27-C28-C29-C39
49	y1	622	XAT	C26-C27-C28-C29
49	y1	622	XAT	C27-C28-C29-C39
50	R	622	NEX	C7-C8-C9-C19
50	R	622	NEX	C12-C13-C14-C15
50	R	622	NEX	C20-C13-C14-C15
50	R	622	NEX	C14-C15-C35-C34
50	S	622	NEX	C11-C10-C9-C8
50	S	622	NEX	C11-C10-C9-C19
50	S	622	NEX	C10-C11-C12-C13
50	S	622	NEX	C11-C12-C13-C14
50	S	622	NEX	C11-C12-C13-C20
50	Y	623	NEX	C28-C29-C30-C31
50	Y	623	NEX	C39-C29-C30-C31
50	g	623	NEX	C28-C29-C30-C31
50	g	623	NEX	C39-C29-C30-C31
50	r	623	NEX	C14-C15-C35-C34
50	s	623	NEX	C10-C11-C12-C13
50	y	623	NEX	O24-C26-C27-C28
50	R1	622	NEX	C12-C13-C14-C15
50	R1	622	NEX	C20-C13-C14-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
50	R1	622	NEX	C14-C15-C35-C34
50	n1	623	NEX	C7-C8-C9-C19
50	r1	622	NEX	C12-C13-C14-C15
50	r1	622	NEX	C20-C13-C14-C15
50	y1	623	NEX	C7-C8-C9-C19
51	S	625	LPX	O1-C3-C4-O5
51	S	625	LPX	C1-O2-P1-O1
51	s	625	LPX	C3-C4-C5-O6
51	s	625	LPX	O1-C3-C4-C5
51	s	625	LPX	C2-C1-O2-P1
51	s1	625	LPX	C3-C4-C5-O6
51	s1	625	LPX	O1-C3-C4-O5
51	s1	625	LPX	C3-O1-P1-O3
51	s1	625	LPX	C3-O1-P1-O2
51	s1	625	LPX	C3-O1-P1-O4
52	S	626	3PH	C22-C21-O21-C2
52	i	101	3PH	C1-O11-P-O13
52	i	101	3PH	C1-O11-P-O14
52	i	101	3PH	C1-O11-P-O12
52	s	626	3PH	C1-O11-P-O13
52	s	626	3PH	C1-O11-P-O14
52	s	626	3PH	C1-O11-P-O12
52	s	626	3PH	O21-C2-C3-O31
52	s	626	3PH	C22-C21-O21-C2
52	T1	101	3PH	C1-O11-P-O13
52	T1	101	3PH	C1-O11-P-O14
52	T1	101	3PH	O22-C21-O21-C2
52	T1	101	3PH	C22-C21-O21-C2
52	S1	626	3PH	C1-O11-P-O13
52	S1	626	3PH	C1-O11-P-O14
52	S1	626	3PH	O22-C21-O21-C2
52	b1	624	3PH	C22-C21-O21-C2
52	b1	624	3PH	O32-C31-O31-C3
52	t1	101	3PH	C1-O11-P-O13
52	t1	101	3PH	C1-O11-P-O14
52	t1	101	3PH	C1-O11-P-O12
52	t1	101	3PH	O22-C21-O21-C2
52	s1	626	3PH	C1-O11-P-O13
52	s1	626	3PH	C1-O11-P-O14
52	s1	626	3PH	O22-C21-O21-C2
53	Y	625	SPH	O1-C1-C2-N2
53	Y	625	SPH	O1-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
53	Y	625	SPH	C1-C2-C3-O3
53	Y	625	SPH	C1-C2-C3-C4
53	Y	625	SPH	N2-C2-C3-C4
53	y	625	SPH	C2-C3-C4-C5
53	A1	414	SPH	O1-C1-C2-N2
53	A1	414	SPH	O1-C1-C2-C3
53	A1	414	SPH	C1-C2-C3-O3
53	A1	414	SPH	C1-C2-C3-C4
53	A1	414	SPH	N2-C2-C3-C4
53	Y1	625	SPH	O1-C1-C2-N2
53	Y1	625	SPH	O1-C1-C2-C3
53	Y1	625	SPH	C2-C3-C4-C5
53	Y1	625	SPH	O3-C3-C4-C5
53	a1	414	SPH	C1-C2-C3-O3
53	a1	414	SPH	C1-C2-C3-C4
53	a1	414	SPH	N2-C2-C3-O3
53	a1	414	SPH	N2-C2-C3-C4
53	y1	625	SPH	O1-C1-C2-N2
53	y1	625	SPH	O1-C1-C2-C3
53	y1	625	SPH	C1-C2-C3-O3
53	y1	625	SPH	C1-C2-C3-C4
53	y1	625	SPH	N2-C2-C3-O3
53	y1	625	SPH	N2-C2-C3-C4
53	y1	625	SPH	C2-C3-C4-C5
53	y1	625	SPH	O3-C3-C4-C5
54	I1	102	4RF	C24-C22-O21-C20
54	i1	101	4RF	O18-C19-C20-O21
54	i1	101	4RF	O21-C20-C39-O40
54	i1	101	4RF	C24-C22-O21-C20
54	i1	101	4RF	O23-C22-O21-C20
56	R1	626	ERG	C13-C17-C20-C21
56	R1	626	ERG	C16-C17-C20-C21
56	r1	626	ERG	C13-C17-C20-C21
56	r1	626	ERG	C16-C17-C20-C21
56	r1	626	ERG	C16-C17-C20-C22
57	Y1	626	PTY	N1-C2-C3-O11
57	Y1	626	PTY	C3-O11-P1-O13
57	Y1	626	PTY	C3-O11-P1-O14
57	Y1	627	PTY	N1-C2-C3-O11
57	Y1	627	PTY	C5-O14-P1-O13
57	y1	626	PTY	C5-O14-P1-O11
57	y1	627	PTY	C3-O11-P1-O12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
57	y1	627	PTY	C3-O11-P1-O13
57	y1	627	PTY	C5-O14-P1-O11
57	y1	627	PTY	C5-O14-P1-O12
57	y1	627	PTY	C5-O14-P1-O13
57	Y1	627	PTY	C11-C8-O7-C6
57	y1	627	PTY	C11-C8-O7-C6
31	N	612	CLA	O1D-CGD-O2D-CED
31	G	613	CLA	O1D-CGD-O2D-CED
31	R	603	CLA	O1D-CGD-O2D-CED
31	R	608	CLA	O1D-CGD-O2D-CED
31	R	609	CLA	O1D-CGD-O2D-CED
31	y	604	CLA	O1D-CGD-O2D-CED
31	y	608	CLA	O1D-CGD-O2D-CED
31	B1	606	CLA	O1D-CGD-O2D-CED
31	R1	604	CLA	O1D-CGD-O2D-CED
31	R1	608	CLA	O1D-CGD-O2D-CED
31	b1	614	CLA	O1D-CGD-O2D-CED
31	c1	502	CLA	O1D-CGD-O2D-CED
31	n1	610	CLA	O1D-CGD-O2D-CED
31	g1	613	CLA	O1D-CGD-O2D-CED
31	r1	604	CLA	O1D-CGD-O2D-CED
31	r1	609	CLA	O1D-CGD-O2D-CED
31	r1	610	CLA	O1D-CGD-O2D-CED
31	s1	617	CLA	O1D-CGD-O2D-CED
57	y1	627	PTY	O10-C8-O7-C6
31	A	405	CLA	O1D-CGD-O2D-CED
31	N	613	CLA	O1D-CGD-O2D-CED
31	a	405	CLA	O1D-CGD-O2D-CED
31	b	606	CLA	O1D-CGD-O2D-CED
31	c	502	CLA	O1D-CGD-O2D-CED
31	n	610	CLA	O1D-CGD-O2D-CED
31	g	610	CLA	O1D-CGD-O2D-CED
31	g	613	CLA	O1D-CGD-O2D-CED
31	r	603	CLA	O1D-CGD-O2D-CED
31	s	609	CLA	O1D-CGD-O2D-CED
31	s	610	CLA	O1D-CGD-O2D-CED
31	B1	604	CLA	O1D-CGD-O2D-CED
31	B1	607	CLA	O1D-CGD-O2D-CED
31	B1	614	CLA	O1D-CGD-O2D-CED
31	B1	615	CLA	O1D-CGD-O2D-CED
31	C1	511	CLA	O1D-CGD-O2D-CED
31	N1	613	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	G1	613	CLA	O1D-CGD-O2D-CED
31	R1	603	CLA	O1D-CGD-O2D-CED
31	S1	613	CLA	O1D-CGD-O2D-CED
31	S1	614	CLA	O1D-CGD-O2D-CED
31	Y1	610	CLA	O1D-CGD-O2D-CED
31	a1	405	CLA	O1D-CGD-O2D-CED
31	b1	604	CLA	O1D-CGD-O2D-CED
31	n1	613	CLA	O1D-CGD-O2D-CED
31	n1	614	CLA	O1D-CGD-O2D-CED
31	g1	610	CLA	O1D-CGD-O2D-CED
31	r1	608	CLA	O1D-CGD-O2D-CED
31	s1	613	CLA	O1D-CGD-O2D-CED
31	y1	611	CLA	O1D-CGD-O2D-CED
31	A	410	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	CBD-CGD-O2D-CED
31	B	606	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	CBD-CGD-O2D-CED
31	B	611	CLA	CBD-CGD-O2D-CED
31	B	613	CLA	CBD-CGD-O2D-CED
31	B	614	CLA	CBD-CGD-O2D-CED
31	B	616	CLA	CBD-CGD-O2D-CED
31	B	617	CLA	CBD-CGD-O2D-CED
31	C	503	CLA	CBD-CGD-O2D-CED
31	C	504	CLA	CBD-CGD-O2D-CED
31	C	507	CLA	CBD-CGD-O2D-CED
31	C	509	CLA	CBD-CGD-O2D-CED
31	C	511	CLA	CBD-CGD-O2D-CED
31	N	602	CLA	CBD-CGD-O2D-CED
31	N	604	CLA	CBD-CGD-O2D-CED
31	N	611	CLA	CBD-CGD-O2D-CED
31	N	612	CLA	CBD-CGD-O2D-CED
31	N	613	CLA	CBD-CGD-O2D-CED
31	G	602	CLA	CBD-CGD-O2D-CED
31	G	604	CLA	CBD-CGD-O2D-CED
31	G	610	CLA	CBD-CGD-O2D-CED
31	G	611	CLA	CBD-CGD-O2D-CED
31	G	612	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	CBD-CGD-O2D-CED
31	R	603	CLA	CBD-CGD-O2D-CED
31	R	604	CLA	CBD-CGD-O2D-CED
31	R	609	CLA	CBD-CGD-O2D-CED
31	R	610	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	612	CLA	CBD-CGD-O2D-CED
31	R	613	CLA	CBD-CGD-O2D-CED
31	S	603	CLA	CBD-CGD-O2D-CED
31	S	604	CLA	CBD-CGD-O2D-CED
31	S	605	CLA	CBD-CGD-O2D-CED
31	S	610	CLA	CBD-CGD-O2D-CED
31	S	613	CLA	CBD-CGD-O2D-CED
31	S	617	CLA	CBD-CGD-O2D-CED
31	Y	602	CLA	CBD-CGD-O2D-CED
31	Y	603	CLA	CBD-CGD-O2D-CED
31	Y	608	CLA	CBD-CGD-O2D-CED
31	Y	610	CLA	CBD-CGD-O2D-CED
31	Y	612	CLA	CBD-CGD-O2D-CED
31	b	602	CLA	CBD-CGD-O2D-CED
31	b	603	CLA	CBD-CGD-O2D-CED
31	b	606	CLA	CBD-CGD-O2D-CED
31	b	607	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	CBD-CGD-O2D-CED
31	b	611	CLA	CBD-CGD-O2D-CED
31	b	613	CLA	CBD-CGD-O2D-CED
31	b	614	CLA	CBD-CGD-O2D-CED
31	b	617	CLA	CBD-CGD-O2D-CED
31	c	503	CLA	CBD-CGD-O2D-CED
31	c	504	CLA	CBD-CGD-O2D-CED
31	c	509	CLA	CBD-CGD-O2D-CED
31	c	511	CLA	CBD-CGD-O2D-CED
31	n	602	CLA	CBD-CGD-O2D-CED
31	n	611	CLA	CBD-CGD-O2D-CED
31	n	613	CLA	CBD-CGD-O2D-CED
31	g	602	CLA	CBD-CGD-O2D-CED
31	g	610	CLA	CBD-CGD-O2D-CED
31	g	611	CLA	CBD-CGD-O2D-CED
31	g	612	CLA	CBD-CGD-O2D-CED
31	g	613	CLA	CBD-CGD-O2D-CED
31	g	614	CLA	CBD-CGD-O2D-CED
31	r	602	CLA	CBD-CGD-O2D-CED
31	r	604	CLA	CBD-CGD-O2D-CED
31	r	608	CLA	CBD-CGD-O2D-CED
31	r	611	CLA	CBD-CGD-O2D-CED
31	r	612	CLA	CBD-CGD-O2D-CED
31	r	613	CLA	CBD-CGD-O2D-CED
31	s	602	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s	609	CLA	CBD-CGD-O2D-CED
31	s	613	CLA	CBD-CGD-O2D-CED
31	s	617	CLA	CBD-CGD-O2D-CED
31	y	602	CLA	CBD-CGD-O2D-CED
31	y	603	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CBD-CGD-O2D-CED
31	y	608	CLA	CBD-CGD-O2D-CED
31	y	610	CLA	CBD-CGD-O2D-CED
31	y	611	CLA	CBD-CGD-O2D-CED
31	y	613	CLA	CBD-CGD-O2D-CED
31	B1	604	CLA	CBD-CGD-O2D-CED
31	B1	606	CLA	CBD-CGD-O2D-CED
31	B1	607	CLA	CBD-CGD-O2D-CED
31	B1	611	CLA	CBD-CGD-O2D-CED
31	B1	612	CLA	CBD-CGD-O2D-CED
31	B1	615	CLA	CBD-CGD-O2D-CED
31	C1	501	CLA	CBD-CGD-O2D-CED
31	C1	502	CLA	CBD-CGD-O2D-CED
31	C1	504	CLA	CBD-CGD-O2D-CED
31	C1	511	CLA	CBD-CGD-O2D-CED
31	D1	403	CLA	CBD-CGD-O2D-CED
31	N1	610	CLA	CBD-CGD-O2D-CED
31	N1	611	CLA	CBD-CGD-O2D-CED
31	N1	613	CLA	CBD-CGD-O2D-CED
31	G1	603	CLA	CBD-CGD-O2D-CED
31	G1	611	CLA	CBD-CGD-O2D-CED
31	G1	613	CLA	CBD-CGD-O2D-CED
31	R1	604	CLA	CBD-CGD-O2D-CED
31	R1	608	CLA	CBD-CGD-O2D-CED
31	S1	603	CLA	CBD-CGD-O2D-CED
31	S1	611	CLA	CBD-CGD-O2D-CED
31	S1	614	CLA	CBD-CGD-O2D-CED
31	Y1	602	CLA	CBD-CGD-O2D-CED
31	Y1	603	CLA	CBD-CGD-O2D-CED
31	Y1	604	CLA	CBD-CGD-O2D-CED
31	Y1	610	CLA	CBD-CGD-O2D-CED
31	Y1	614	CLA	CBD-CGD-O2D-CED
31	a1	407	CLA	CBD-CGD-O2D-CED
31	a1	410	CLA	CBD-CGD-O2D-CED
31	b1	602	CLA	CBD-CGD-O2D-CED
31	b1	603	CLA	CBD-CGD-O2D-CED
31	b1	604	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b1	606	CLA	CBD-CGD-O2D-CED
31	b1	609	CLA	CBD-CGD-O2D-CED
31	b1	610	CLA	CBD-CGD-O2D-CED
31	b1	613	CLA	CBD-CGD-O2D-CED
31	b1	615	CLA	CBD-CGD-O2D-CED
31	c1	501	CLA	CBD-CGD-O2D-CED
31	c1	502	CLA	CBD-CGD-O2D-CED
31	c1	503	CLA	CBD-CGD-O2D-CED
31	c1	507	CLA	CBD-CGD-O2D-CED
31	c1	509	CLA	CBD-CGD-O2D-CED
31	c1	510	CLA	CBD-CGD-O2D-CED
31	c1	511	CLA	CBD-CGD-O2D-CED
31	n1	602	CLA	CBD-CGD-O2D-CED
31	n1	604	CLA	CBD-CGD-O2D-CED
31	n1	610	CLA	CBD-CGD-O2D-CED
31	n1	611	CLA	CBD-CGD-O2D-CED
31	n1	612	CLA	CBD-CGD-O2D-CED
31	n1	613	CLA	CBD-CGD-O2D-CED
31	n1	614	CLA	CBD-CGD-O2D-CED
31	g1	602	CLA	CBD-CGD-O2D-CED
31	g1	603	CLA	CBD-CGD-O2D-CED
31	g1	613	CLA	CBD-CGD-O2D-CED
31	g1	614	CLA	CBD-CGD-O2D-CED
31	r1	604	CLA	CBD-CGD-O2D-CED
31	r1	610	CLA	CBD-CGD-O2D-CED
31	s1	602	CLA	CBD-CGD-O2D-CED
31	s1	604	CLA	CBD-CGD-O2D-CED
31	s1	605	CLA	CBD-CGD-O2D-CED
31	s1	609	CLA	CBD-CGD-O2D-CED
31	s1	610	CLA	CBD-CGD-O2D-CED
31	s1	612	CLA	CBD-CGD-O2D-CED
31	s1	614	CLA	CBD-CGD-O2D-CED
31	s1	617	CLA	CBD-CGD-O2D-CED
31	y1	603	CLA	CBD-CGD-O2D-CED
31	y1	604	CLA	CBD-CGD-O2D-CED
31	y1	608	CLA	CBD-CGD-O2D-CED
31	y1	611	CLA	CBD-CGD-O2D-CED
31	y1	612	CLA	CBD-CGD-O2D-CED
31	y1	614	CLA	CBD-CGD-O2D-CED
32	a	409	PHO	CBD-CGD-O2D-CED
31	B	617	CLA	O1A-CGA-O2A-C1
31	C	504	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N	611	CLA	O1A-CGA-O2A-C1
31	S	603	CLA	O1A-CGA-O2A-C1
31	S	605	CLA	O1A-CGA-O2A-C1
31	c	512	CLA	O1A-CGA-O2A-C1
31	g	614	CLA	O1A-CGA-O2A-C1
31	s	605	CLA	O1A-CGA-O2A-C1
31	y	603	CLA	O1A-CGA-O2A-C1
31	y	611	CLA	O1A-CGA-O2A-C1
31	A1	406	CLA	O1A-CGA-O2A-C1
31	C1	505	CLA	O1A-CGA-O2A-C1
31	G1	611	CLA	O1A-CGA-O2A-C1
31	G1	614	CLA	O1A-CGA-O2A-C1
31	S1	605	CLA	O1A-CGA-O2A-C1
31	S1	613	CLA	O1A-CGA-O2A-C1
31	Y1	611	CLA	O1A-CGA-O2A-C1
31	d1	403	CLA	O1A-CGA-O2A-C1
31	g1	611	CLA	O1A-CGA-O2A-C1
31	s1	605	CLA	O1A-CGA-O2A-C1
31	s1	610	CLA	O1A-CGA-O2A-C1
31	y1	612	CLA	O1A-CGA-O2A-C1
52	t1	101	3PH	O32-C31-O31-C3
54	i1	101	4RF	O17-C16-O18-C19
31	R	613	CLA	O1A-CGA-O2A-C1
31	B	602	CLA	O1D-CGD-O2D-CED
31	B	604	CLA	O1D-CGD-O2D-CED
31	B	606	CLA	O1D-CGD-O2D-CED
31	B	614	CLA	O1D-CGD-O2D-CED
31	B	617	CLA	O1D-CGD-O2D-CED
31	C	503	CLA	O1D-CGD-O2D-CED
31	C	511	CLA	O1D-CGD-O2D-CED
31	R	610	CLA	O1D-CGD-O2D-CED
31	S	617	CLA	O1D-CGD-O2D-CED
31	Y	608	CLA	O1D-CGD-O2D-CED
31	b	602	CLA	O1D-CGD-O2D-CED
31	b	610	CLA	O1D-CGD-O2D-CED
31	b	614	CLA	O1D-CGD-O2D-CED
31	b	617	CLA	O1D-CGD-O2D-CED
31	c	504	CLA	O1D-CGD-O2D-CED
31	d	403	CLA	O1D-CGD-O2D-CED
31	n	613	CLA	O1D-CGD-O2D-CED
31	g	614	CLA	O1D-CGD-O2D-CED
31	r	611	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s	617	CLA	O1D-CGD-O2D-CED
31	y	610	CLA	O1D-CGD-O2D-CED
31	A1	405	CLA	O1D-CGD-O2D-CED
31	C1	501	CLA	O1D-CGD-O2D-CED
31	C1	506	CLA	O1D-CGD-O2D-CED
31	D1	402	CLA	O1D-CGD-O2D-CED
31	N1	610	CLA	O1D-CGD-O2D-CED
31	G1	603	CLA	O1D-CGD-O2D-CED
31	b1	602	CLA	O1D-CGD-O2D-CED
31	b1	606	CLA	O1D-CGD-O2D-CED
31	b1	610	CLA	O1D-CGD-O2D-CED
31	b1	615	CLA	O1D-CGD-O2D-CED
31	c1	503	CLA	O1D-CGD-O2D-CED
31	c1	504	CLA	O1D-CGD-O2D-CED
31	c1	512	CLA	O1D-CGD-O2D-CED
31	s1	610	CLA	O1D-CGD-O2D-CED
31	y1	608	CLA	O1D-CGD-O2D-CED
31	y1	614	CLA	O1D-CGD-O2D-CED
31	B	610	CLA	O1D-CGD-O2D-CED
31	D	402	CLA	O1D-CGD-O2D-CED
31	N	614	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	O1D-CGD-O2D-CED
31	S	603	CLA	O1D-CGD-O2D-CED
31	S	609	CLA	O1D-CGD-O2D-CED
31	S	613	CLA	O1D-CGD-O2D-CED
31	Y	614	CLA	O1D-CGD-O2D-CED
31	b	612	CLA	O1D-CGD-O2D-CED
31	c	503	CLA	O1D-CGD-O2D-CED
31	c	511	CLA	O1D-CGD-O2D-CED
31	n	614	CLA	O1D-CGD-O2D-CED
31	g	603	CLA	O1D-CGD-O2D-CED
31	g	604	CLA	O1D-CGD-O2D-CED
31	g	611	CLA	O1D-CGD-O2D-CED
31	r	608	CLA	O1D-CGD-O2D-CED
31	r	609	CLA	O1D-CGD-O2D-CED
31	s	603	CLA	O1D-CGD-O2D-CED
31	s	611	CLA	O1D-CGD-O2D-CED
31	s	612	CLA	O1D-CGD-O2D-CED
31	y	613	CLA	O1D-CGD-O2D-CED
31	B1	603	CLA	O1D-CGD-O2D-CED
31	C1	509	CLA	O1D-CGD-O2D-CED
31	C1	510	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C1	512	CLA	O1D-CGD-O2D-CED
31	C1	513	CLA	O1D-CGD-O2D-CED
31	N1	603	CLA	O1D-CGD-O2D-CED
31	G1	614	CLA	O1D-CGD-O2D-CED
31	R1	609	CLA	O1D-CGD-O2D-CED
31	R1	612	CLA	O1D-CGD-O2D-CED
31	S1	609	CLA	O1D-CGD-O2D-CED
31	S1	611	CLA	O1D-CGD-O2D-CED
31	S1	617	CLA	O1D-CGD-O2D-CED
31	Y1	608	CLA	O1D-CGD-O2D-CED
31	Y1	613	CLA	O1D-CGD-O2D-CED
31	b1	608	CLA	O1D-CGD-O2D-CED
31	c1	513	CLA	O1D-CGD-O2D-CED
31	d1	403	CLA	O1D-CGD-O2D-CED
31	g1	604	CLA	O1D-CGD-O2D-CED
31	g1	611	CLA	O1D-CGD-O2D-CED
31	r1	612	CLA	O1D-CGD-O2D-CED
31	s1	611	CLA	O1D-CGD-O2D-CED
31	s1	614	CLA	O1D-CGD-O2D-CED
31	y1	610	CLA	O1D-CGD-O2D-CED
31	B	617	CLA	CBA-CGA-O2A-C1
31	C	504	CLA	CBA-CGA-O2A-C1
31	C	505	CLA	CBA-CGA-O2A-C1
31	g	614	CLA	CBA-CGA-O2A-C1
31	s	605	CLA	CBA-CGA-O2A-C1
31	A1	406	CLA	CBA-CGA-O2A-C1
31	C1	505	CLA	CBA-CGA-O2A-C1
31	G1	611	CLA	CBA-CGA-O2A-C1
31	S1	605	CLA	CBA-CGA-O2A-C1
31	g1	611	CLA	CBA-CGA-O2A-C1
31	y1	604	CLA	CBA-CGA-O2A-C1
35	C1	521	LMG	C29-C28-O8-C9
54	i1	101	4RF	C15-C16-O18-C19
31	C	501	CLA	CBD-CGD-O2D-CED
31	C	502	CLA	CBD-CGD-O2D-CED
31	C	506	CLA	CBD-CGD-O2D-CED
31	C	510	CLA	CBD-CGD-O2D-CED
31	C	513	CLA	CBD-CGD-O2D-CED
31	N	603	CLA	CBD-CGD-O2D-CED
31	N	610	CLA	CBD-CGD-O2D-CED
31	R	602	CLA	CBD-CGD-O2D-CED
31	S	612	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	S	614	CLA	CBD-CGD-O2D-CED
31	a	410	CLA	CBD-CGD-O2D-CED
31	b	609	CLA	CBD-CGD-O2D-CED
31	b	616	CLA	CBD-CGD-O2D-CED
31	c	501	CLA	CBD-CGD-O2D-CED
31	c	506	CLA	CBD-CGD-O2D-CED
31	c	507	CLA	CBD-CGD-O2D-CED
31	c	510	CLA	CBD-CGD-O2D-CED
31	c	513	CLA	CBD-CGD-O2D-CED
31	r	610	CLA	CBD-CGD-O2D-CED
31	s	605	CLA	CBD-CGD-O2D-CED
31	y	612	CLA	CBD-CGD-O2D-CED
31	y	614	CLA	CBD-CGD-O2D-CED
31	A1	407	CLA	CBD-CGD-O2D-CED
31	A1	410	CLA	CBD-CGD-O2D-CED
31	B1	609	CLA	CBD-CGD-O2D-CED
31	B1	613	CLA	CBD-CGD-O2D-CED
31	C1	507	CLA	CBD-CGD-O2D-CED
31	N1	604	CLA	CBD-CGD-O2D-CED
31	N1	612	CLA	CBD-CGD-O2D-CED
31	G1	612	CLA	CBD-CGD-O2D-CED
31	R1	602	CLA	CBD-CGD-O2D-CED
31	S1	602	CLA	CBD-CGD-O2D-CED
31	S1	612	CLA	CBD-CGD-O2D-CED
31	Y1	612	CLA	CBD-CGD-O2D-CED
31	d1	402	CLA	CBD-CGD-O2D-CED
31	n1	603	CLA	CBD-CGD-O2D-CED
31	g1	612	CLA	CBD-CGD-O2D-CED
31	r1	602	CLA	CBD-CGD-O2D-CED
31	s1	603	CLA	CBD-CGD-O2D-CED
31	A1	405	CLA	C2C-C3C-CAC-CBC
31	A1	405	CLA	C4C-C3C-CAC-CBC
31	A	406	CLA	O1A-CGA-O2A-C1
31	B	603	CLA	O1A-CGA-O2A-C1
31	C	505	CLA	O1A-CGA-O2A-C1
31	G	602	CLA	O1A-CGA-O2A-C1
31	G	613	CLA	O1A-CGA-O2A-C1
31	G	614	CLA	O1A-CGA-O2A-C1
31	S	609	CLA	O1A-CGA-O2A-C1
31	S	613	CLA	O1A-CGA-O2A-C1
31	Y	603	CLA	O1A-CGA-O2A-C1
31	Y	604	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	Y	611	CLA	O1A-CGA-O2A-C1
31	a	406	CLA	O1A-CGA-O2A-C1
31	b	603	CLA	O1A-CGA-O2A-C1
31	c	505	CLA	O1A-CGA-O2A-C1
31	d	403	CLA	O1A-CGA-O2A-C1
31	g	604	CLA	O1A-CGA-O2A-C1
31	g	613	CLA	O1A-CGA-O2A-C1
31	s	603	CLA	O1A-CGA-O2A-C1
31	y	604	CLA	O1A-CGA-O2A-C1
31	B1	611	CLA	O1A-CGA-O2A-C1
31	G1	602	CLA	O1A-CGA-O2A-C1
31	G1	604	CLA	O1A-CGA-O2A-C1
31	R1	603	CLA	O1A-CGA-O2A-C1
31	S1	609	CLA	O1A-CGA-O2A-C1
31	S1	610	CLA	O1A-CGA-O2A-C1
31	S1	617	CLA	O1A-CGA-O2A-C1
31	Y1	604	CLA	O1A-CGA-O2A-C1
31	a1	406	CLA	O1A-CGA-O2A-C1
31	b1	603	CLA	O1A-CGA-O2A-C1
31	c1	511	CLA	O1A-CGA-O2A-C1
31	n1	611	CLA	O1A-CGA-O2A-C1
31	g1	602	CLA	O1A-CGA-O2A-C1
31	g1	604	CLA	O1A-CGA-O2A-C1
31	r1	603	CLA	O1A-CGA-O2A-C1
31	s1	603	CLA	O1A-CGA-O2A-C1
31	s1	604	CLA	O1A-CGA-O2A-C1
31	y1	604	CLA	O1A-CGA-O2A-C1
31	y1	611	CLA	O1A-CGA-O2A-C1
32	A	408	PHO	O1A-CGA-O2A-C1
34	c1	526	SQD	O10-C23-O48-C46
35	J	101	LMG	O10-C28-O8-C9
35	c	521	LMG	O10-C28-O8-C9
35	C1	521	LMG	O10-C28-O8-C9
35	C1	523	LMG	O10-C28-O8-C9
35	W1	201	LMG	O10-C28-O8-C9
35	c1	521	LMG	O10-C28-O8-C9
35	w1	201	LMG	O10-C28-O8-C9
52	S	626	3PH	O32-C31-O31-C3
52	i	101	3PH	O32-C31-O31-C3
52	s	626	3PH	O32-C31-O31-C3
31	r	611	CLA	O1A-CGA-O2A-C1
31	D	403	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	611	CLA	O1D-CGD-O2D-CED
31	Y	613	CLA	O1D-CGD-O2D-CED
31	b	604	CLA	O1D-CGD-O2D-CED
31	n	603	CLA	O1D-CGD-O2D-CED
31	B1	610	CLA	O1D-CGD-O2D-CED
31	N1	614	CLA	O1D-CGD-O2D-CED
31	G1	604	CLA	O1D-CGD-O2D-CED
31	R1	610	CLA	O1D-CGD-O2D-CED
31	S1	605	CLA	O1D-CGD-O2D-CED
31	S1	610	CLA	O1D-CGD-O2D-CED
31	b1	612	CLA	O1D-CGD-O2D-CED
31	r1	603	CLA	O1D-CGD-O2D-CED
31	y1	613	CLA	O1D-CGD-O2D-CED
32	a1	409	PHO	O1D-CGD-O2D-CED
57	Y1	627	PTY	O10-C8-O7-C6
55	r1	625	LMT	O5B-C5B-C6B-O6B
31	B	608	CLA	O1D-CGD-O2D-CED
31	G	603	CLA	O1D-CGD-O2D-CED
31	G	612	CLA	O1D-CGD-O2D-CED
31	G	614	CLA	O1D-CGD-O2D-CED
31	S	611	CLA	O1D-CGD-O2D-CED
31	c	509	CLA	O1D-CGD-O2D-CED
31	n	612	CLA	O1D-CGD-O2D-CED
31	s	604	CLA	O1D-CGD-O2D-CED
31	B1	608	CLA	O1D-CGD-O2D-CED
31	B1	616	CLA	O1D-CGD-O2D-CED
31	B1	617	CLA	O1D-CGD-O2D-CED
31	C1	503	CLA	O1D-CGD-O2D-CED
31	N1	602	CLA	O1D-CGD-O2D-CED
31	G1	602	CLA	O1D-CGD-O2D-CED
31	Y1	611	CLA	O1D-CGD-O2D-CED
31	b1	607	CLA	O1D-CGD-O2D-CED
31	b1	611	CLA	O1D-CGD-O2D-CED
31	b1	616	CLA	O1D-CGD-O2D-CED
31	b1	617	CLA	O1D-CGD-O2D-CED
31	y1	602	CLA	O1D-CGD-O2D-CED
31	B	609	CLA	CBD-CGD-O2D-CED
32	a	408	PHO	CBD-CGD-O2D-CED
31	B	611	CLA	O1D-CGD-O2D-CED
31	Y	612	CLA	O1D-CGD-O2D-CED
31	n	602	CLA	O1D-CGD-O2D-CED
31	r	602	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	r	613	CLA	O1D-CGD-O2D-CED
31	B1	611	CLA	O1D-CGD-O2D-CED
31	C1	502	CLA	O1D-CGD-O2D-CED
31	S1	604	CLA	O1D-CGD-O2D-CED
31	Y1	604	CLA	O1D-CGD-O2D-CED
31	c1	501	CLA	O1D-CGD-O2D-CED
31	c1	510	CLA	O1D-CGD-O2D-CED
31	y1	612	CLA	O1D-CGD-O2D-CED
35	A	413	LMG	O9-C10-O7-C8
35	B	622	LMG	O9-C10-O7-C8
35	C	521	LMG	O9-C10-O7-C8
35	W1	201	LMG	O9-C10-O7-C8
35	c1	521	LMG	O9-C10-O7-C8
38	B	625	DGA	OB1-CB1-OG2-CG2
38	b	623	DGA	OB1-CB1-OG2-CG2
40	C	520	DGD	O1B-C1B-O2G-C2G
40	B1	623	DGD	O1B-C1B-O2G-C2G
41	G	630	LHG	O9-C7-O7-C5
41	S	624	LHG	O9-C7-O7-C5
41	d	408	LHG	O9-C7-O7-C5
41	n1	624	LHG	O9-C7-O7-C5
52	S	626	3PH	O22-C21-O21-C2
52	s	626	3PH	O22-C21-O21-C2
52	b1	624	3PH	O22-C21-O21-C2
54	I1	102	4RF	O23-C22-O21-C20
31	N	604	CLA	O1D-CGD-O2D-CED
31	C	512	CLA	C3-C5-C6-C7
31	D	403	CLA	C3-C5-C6-C7
31	N	603	CLA	C3-C5-C6-C7
31	Y	610	CLA	C3-C5-C6-C7
31	Y	613	CLA	C3-C5-C6-C7
31	Y	614	CLA	C3-C5-C6-C7
31	a	405	CLA	C3-C5-C6-C7
31	b	605	CLA	C3-C5-C6-C7
31	b	610	CLA	C3-C5-C6-C7
31	b	612	CLA	C3-C5-C6-C7
31	c	503	CLA	C3-C5-C6-C7
31	d	403	CLA	C3-C5-C6-C7
31	n	602	CLA	C3-C5-C6-C7
31	r	609	CLA	C3-C5-C6-C7
31	y	614	CLA	C3-C5-C6-C7
31	A1	406	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B1	604	CLA	C3-C5-C6-C7
31	B1	608	CLA	C3-C5-C6-C7
31	B1	610	CLA	C3-C5-C6-C7
31	C1	505	CLA	C3-C5-C6-C7
31	C1	506	CLA	C3-C5-C6-C7
31	S1	603	CLA	C3-C5-C6-C7
31	S1	604	CLA	C3-C5-C6-C7
31	S1	610	CLA	C3-C5-C6-C7
31	b1	602	CLA	C3-C5-C6-C7
31	b1	614	CLA	C3-C5-C6-C7
31	b1	617	CLA	C3-C5-C6-C7
31	c1	504	CLA	C3-C5-C6-C7
31	d1	403	CLA	C3-C5-C6-C7
31	n1	604	CLA	C3-C5-C6-C7
31	n1	610	CLA	C3-C5-C6-C7
31	g1	611	CLA	C3-C5-C6-C7
31	r1	608	CLA	C3-C5-C6-C7
31	s1	603	CLA	C3-C5-C6-C7
31	s1	609	CLA	C3-C5-C6-C7
31	s1	610	CLA	C3-C5-C6-C7
31	y1	611	CLA	C3-C5-C6-C7
32	A	408	PHO	C3-C5-C6-C7
32	A	409	PHO	C3-C5-C6-C7
32	a	409	PHO	C3-C5-C6-C7
32	A1	408	PHO	C3-C5-C6-C7
47	Y1	607	CHL	C3-C5-C6-C7
31	A	410	CLA	CBA-CGA-O2A-C1
31	B	603	CLA	CBA-CGA-O2A-C1
31	B	608	CLA	CBA-CGA-O2A-C1
31	C	511	CLA	CBA-CGA-O2A-C1
31	C	512	CLA	CBA-CGA-O2A-C1
31	N	611	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	CBA-CGA-O2A-C1
31	G	614	CLA	CBA-CGA-O2A-C1
31	R	608	CLA	CBA-CGA-O2A-C1
31	R	612	CLA	CBA-CGA-O2A-C1
31	S	603	CLA	CBA-CGA-O2A-C1
31	S	605	CLA	CBA-CGA-O2A-C1
31	Y	604	CLA	CBA-CGA-O2A-C1
31	Y	611	CLA	CBA-CGA-O2A-C1
31	Y	613	CLA	CBA-CGA-O2A-C1
31	a	406	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b	603	CLA	CBA-CGA-O2A-C1
31	b	605	CLA	CBA-CGA-O2A-C1
31	c	505	CLA	CBA-CGA-O2A-C1
31	c	512	CLA	CBA-CGA-O2A-C1
31	d	403	CLA	CBA-CGA-O2A-C1
31	g	613	CLA	CBA-CGA-O2A-C1
31	s	602	CLA	CBA-CGA-O2A-C1
31	s	603	CLA	CBA-CGA-O2A-C1
31	y	603	CLA	CBA-CGA-O2A-C1
31	y	604	CLA	CBA-CGA-O2A-C1
31	y	611	CLA	CBA-CGA-O2A-C1
31	y	612	CLA	CBA-CGA-O2A-C1
31	B1	603	CLA	CBA-CGA-O2A-C1
31	C1	511	CLA	CBA-CGA-O2A-C1
31	G1	602	CLA	CBA-CGA-O2A-C1
31	R1	603	CLA	CBA-CGA-O2A-C1
31	R1	609	CLA	CBA-CGA-O2A-C1
31	S1	613	CLA	CBA-CGA-O2A-C1
31	Y1	602	CLA	CBA-CGA-O2A-C1
31	Y1	604	CLA	CBA-CGA-O2A-C1
31	Y1	611	CLA	CBA-CGA-O2A-C1
31	a1	406	CLA	CBA-CGA-O2A-C1
31	b1	606	CLA	CBA-CGA-O2A-C1
31	n1	611	CLA	CBA-CGA-O2A-C1
31	r1	603	CLA	CBA-CGA-O2A-C1
31	s1	604	CLA	CBA-CGA-O2A-C1
31	s1	610	CLA	CBA-CGA-O2A-C1
31	y1	611	CLA	CBA-CGA-O2A-C1
31	y1	612	CLA	CBA-CGA-O2A-C1
32	A	408	PHO	CBA-CGA-O2A-C1
34	c1	526	SQD	C24-C23-O48-C46
35	J	101	LMG	C29-C28-O8-C9
35	c	521	LMG	C29-C28-O8-C9
35	W1	201	LMG	C29-C28-O8-C9
35	w1	201	LMG	C29-C28-O8-C9
52	s	626	3PH	C32-C31-O31-C3
52	b1	624	3PH	C32-C31-O31-C3
52	t1	101	3PH	C32-C31-O31-C3
57	y1	626	PTY	C31-C30-O4-C1
57	Y1	627	PTY	O30-C30-O4-C1
35	b	622	LMG	C11-C10-O7-C8
35	c	521	LMG	C11-C10-O7-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	B1	622	LMG	C11-C10-O7-C8
35	c1	521	LMG	C11-C10-O7-C8
38	B	625	DGA	CB2-CB1-OG2-CG2
40	C	523	DGD	C2B-C1B-O2G-C2G
41	N	624	LHG	C8-C7-O7-C5
41	n	624	LHG	C8-C7-O7-C5
52	t1	101	3PH	C22-C21-O21-C2
31	G	611	CLA	O1D-CGD-O2D-CED
31	R	613	CLA	O1D-CGD-O2D-CED
31	Y	610	CLA	O1D-CGD-O2D-CED
31	r	604	CLA	O1D-CGD-O2D-CED
31	s	602	CLA	O1D-CGD-O2D-CED
31	S1	603	CLA	O1D-CGD-O2D-CED
31	Y1	614	CLA	O1D-CGD-O2D-CED
31	c1	509	CLA	O1D-CGD-O2D-CED
31	n1	612	CLA	O1D-CGD-O2D-CED
31	g1	614	CLA	O1D-CGD-O2D-CED
31	s1	612	CLA	O1D-CGD-O2D-CED
31	s	614	CLA	CBD-CGD-O2D-CED
31	S	602	CLA	O1A-CGA-O2A-C1
31	N1	611	CLA	O1A-CGA-O2A-C1
31	C	513	CLA	C4-C3-C5-C6
31	b	604	CLA	C4-C3-C5-C6
31	b	606	CLA	C4-C3-C5-C6
31	c	501	CLA	C4-C3-C5-C6
31	c	503	CLA	C4-C3-C5-C6
31	C1	503	CLA	C4-C3-C5-C6
31	C1	505	CLA	C4-C3-C5-C6
31	c1	504	CLA	C4-C3-C5-C6
31	r1	610	CLA	C4-C3-C5-C6
47	G	609	CHL	C4-C3-C5-C6
47	Y	606	CHL	C4-C3-C5-C6
31	b	606	CLA	C2-C3-C5-C6
31	b	607	CLA	C2-C3-C5-C6
31	b	612	CLA	C2-C3-C5-C6
31	c1	501	CLA	C2-C3-C5-C6
47	y	601	CHL	C2-C3-C5-C6
47	g1	609	CHL	C2-C3-C5-C6
31	C	508	CLA	CBD-CGD-O2D-CED
31	C1	508	CLA	CBD-CGD-O2D-CED
31	N	614	CLA	C2A-CAA-CBA-CGA
31	G	613	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	603	CLA	C2A-CAA-CBA-CGA
31	R	609	CLA	C2A-CAA-CBA-CGA
31	S	614	CLA	C2A-CAA-CBA-CGA
31	b	602	CLA	C2A-CAA-CBA-CGA
31	b	612	CLA	C2A-CAA-CBA-CGA
31	c	504	CLA	C2A-CAA-CBA-CGA
31	g	613	CLA	C2A-CAA-CBA-CGA
31	r	602	CLA	C2A-CAA-CBA-CGA
31	A1	407	CLA	C2A-CAA-CBA-CGA
31	C1	502	CLA	C2A-CAA-CBA-CGA
31	R1	609	CLA	C2A-CAA-CBA-CGA
31	S1	602	CLA	C2A-CAA-CBA-CGA
31	Y1	613	CLA	C2A-CAA-CBA-CGA
31	a1	407	CLA	C2A-CAA-CBA-CGA
31	b1	603	CLA	C2A-CAA-CBA-CGA
31	b1	604	CLA	C2A-CAA-CBA-CGA
31	c1	507	CLA	C2A-CAA-CBA-CGA
31	g1	613	CLA	C2A-CAA-CBA-CGA
31	g1	614	CLA	C2A-CAA-CBA-CGA
31	r1	609	CLA	C2A-CAA-CBA-CGA
31	s1	602	CLA	C2A-CAA-CBA-CGA
31	y1	608	CLA	C2A-CAA-CBA-CGA
47	N	605	CHL	C2A-CAA-CBA-CGA
47	n	609	CHL	C2A-CAA-CBA-CGA
47	g	606	CHL	C2A-CAA-CBA-CGA
47	y	605	CHL	C2A-CAA-CBA-CGA
47	N1	605	CHL	C2A-CAA-CBA-CGA
47	G1	605	CHL	C2A-CAA-CBA-CGA
47	Y1	605	CHL	C2A-CAA-CBA-CGA
47	Y1	607	CHL	C2A-CAA-CBA-CGA
47	n1	606	CHL	C2A-CAA-CBA-CGA
47	n1	608	CHL	C2A-CAA-CBA-CGA
47	g1	601	CHL	C2A-CAA-CBA-CGA
47	s1	601	CHL	C2A-CAA-CBA-CGA
47	y1	605	CHL	C2A-CAA-CBA-CGA
31	r	609	CLA	O1A-CGA-O2A-C1
31	N1	603	CLA	O1A-CGA-O2A-C1
31	y1	608	CLA	O1A-CGA-O2A-C1
54	I1	102	4RF	O17-C16-O18-C19
31	b	607	CLA	O1D-CGD-O2D-CED
35	A	413	LMG	C17-C18-C19-C20
35	A	413	LMG	C35-C36-C37-C38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	A	413	LMG	C38-C39-C40-C41
35	B	622	LMG	C17-C18-C19-C20
35	C	521	LMG	C17-C18-C19-C20
35	C	521	LMG	C35-C36-C37-C38
35	D	411	LMG	C17-C18-C19-C20
35	D	411	LMG	C20-C21-C22-C23
35	H	102	LMG	C38-C39-C40-C41
35	J	101	LMG	C17-C18-C19-C20
35	J	101	LMG	C20-C21-C22-C23
35	a	413	LMG	C17-C18-C19-C20
35	a	413	LMG	C35-C36-C37-C38
35	a	413	LMG	C38-C39-C40-C41
35	b	622	LMG	C17-C18-C19-C20
35	c	521	LMG	C17-C18-C19-C20
35	c	521	LMG	C35-C36-C37-C38
35	d	411	LMG	C17-C18-C19-C20
35	d	411	LMG	C20-C21-C22-C23
35	h	102	LMG	C38-C39-C40-C41
35	j	101	LMG	C17-C18-C19-C20
35	j	101	LMG	C20-C21-C22-C23
35	A1	413	LMG	C17-C18-C19-C20
35	A1	413	LMG	C35-C36-C37-C38
35	A1	413	LMG	C38-C39-C40-C41
35	B1	622	LMG	C17-C18-C19-C20
35	C1	521	LMG	C17-C18-C19-C20
35	C1	521	LMG	C35-C36-C37-C38
35	C1	523	LMG	C17-C18-C19-C20
35	C1	523	LMG	C41-C42-C43-C44
35	D1	411	LMG	C17-C18-C19-C20
35	D1	411	LMG	C20-C21-C22-C23
35	H1	102	LMG	C38-C39-C40-C41
35	W1	201	LMG	C35-C36-C37-C38
35	W1	201	LMG	C38-C39-C40-C41
35	a1	413	LMG	C17-C18-C19-C20
35	a1	413	LMG	C35-C36-C37-C38
35	a1	413	LMG	C38-C39-C40-C41
35	b1	622	LMG	C17-C18-C19-C20
35	c1	521	LMG	C17-C18-C19-C20
35	c1	521	LMG	C35-C36-C37-C38
35	c1	523	LMG	C17-C18-C19-C20
35	c1	523	LMG	C41-C42-C43-C44
35	d1	411	LMG	C17-C18-C19-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	h1	102	LMG	C38-C39-C40-C41
35	w1	201	LMG	C35-C36-C37-C38
35	w1	201	LMG	C38-C39-C40-C41
40	C	518	DGD	C8B-C9B-CAB-CBB
40	C	519	DGD	C8A-C9A-CAA-CBA
40	C	519	DGD	C8B-C9B-CAB-CBB
40	C	520	DGD	CBB-CCB-CDB-CEB
40	C	523	DGD	CBA-CCA-CDA-CEA
40	C	523	DGD	CEB-CFB-CGB-CHB
40	c	518	DGD	C8B-C9B-CAB-CBB
40	c	519	DGD	C8A-C9A-CAA-CBA
40	c	519	DGD	C8B-C9B-CAB-CBB
40	c	520	DGD	CBB-CCB-CDB-CEB
40	c	523	DGD	CBA-CCA-CDA-CEA
40	c	523	DGD	CEB-CFB-CGB-CHB
40	C1	518	DGD	C8B-C9B-CAB-CBB
40	C1	519	DGD	C8A-C9A-CAA-CBA
40	C1	519	DGD	CBB-CCB-CDB-CEB
40	C1	520	DGD	CBB-CCB-CDB-CEB
40	c1	518	DGD	C8B-C9B-CAB-CBB
40	c1	519	DGD	C8A-C9A-CAA-CBA
40	c1	519	DGD	CBB-CCB-CDB-CEB
40	c1	520	DGD	CBB-CCB-CDB-CEB
31	B	605	CLA	C3-C5-C6-C7
31	B	612	CLA	C3-C5-C6-C7
31	C	504	CLA	C3-C5-C6-C7
31	C	510	CLA	C3-C5-C6-C7
31	N	610	CLA	C3-C5-C6-C7
31	G	603	CLA	C3-C5-C6-C7
31	b	608	CLA	C3-C5-C6-C7
31	n	613	CLA	C3-C5-C6-C7
31	s	611	CLA	C3-C5-C6-C7
31	y	611	CLA	C3-C5-C6-C7
31	B1	609	CLA	C3-C5-C6-C7
31	B1	614	CLA	C3-C5-C6-C7
31	G1	611	CLA	C3-C5-C6-C7
31	R1	602	CLA	C3-C5-C6-C7
31	S1	609	CLA	C3-C5-C6-C7
31	Y1	604	CLA	C3-C5-C6-C7
31	c1	505	CLA	C3-C5-C6-C7
31	c1	506	CLA	C3-C5-C6-C7
31	n1	613	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s1	604	CLA	C3-C5-C6-C7
32	A1	409	PHO	C3-C5-C6-C7
32	a1	409	PHO	C3-C5-C6-C7
31	A	406	CLA	CBA-CGA-O2A-C1
31	C	510	CLA	CBA-CGA-O2A-C1
31	D	403	CLA	CBA-CGA-O2A-C1
31	G	602	CLA	CBA-CGA-O2A-C1
31	G	613	CLA	CBA-CGA-O2A-C1
31	R	603	CLA	CBA-CGA-O2A-C1
31	R	609	CLA	CBA-CGA-O2A-C1
31	S	609	CLA	CBA-CGA-O2A-C1
31	S	613	CLA	CBA-CGA-O2A-C1
31	Y	603	CLA	CBA-CGA-O2A-C1
31	Y	612	CLA	CBA-CGA-O2A-C1
31	a	405	CLA	CBA-CGA-O2A-C1
31	b	602	CLA	CBA-CGA-O2A-C1
31	b	608	CLA	CBA-CGA-O2A-C1
31	c	511	CLA	CBA-CGA-O2A-C1
31	g	604	CLA	CBA-CGA-O2A-C1
31	r	603	CLA	CBA-CGA-O2A-C1
31	r	608	CLA	CBA-CGA-O2A-C1
31	r	609	CLA	CBA-CGA-O2A-C1
31	r	612	CLA	CBA-CGA-O2A-C1
31	s	613	CLA	CBA-CGA-O2A-C1
31	y	614	CLA	CBA-CGA-O2A-C1
31	B1	611	CLA	CBA-CGA-O2A-C1
31	B1	613	CLA	CBA-CGA-O2A-C1
31	C1	506	CLA	CBA-CGA-O2A-C1
31	C1	509	CLA	CBA-CGA-O2A-C1
31	C1	513	CLA	CBA-CGA-O2A-C1
31	G1	604	CLA	CBA-CGA-O2A-C1
31	G1	613	CLA	CBA-CGA-O2A-C1
31	S1	602	CLA	CBA-CGA-O2A-C1
31	S1	609	CLA	CBA-CGA-O2A-C1
31	S1	610	CLA	CBA-CGA-O2A-C1
31	S1	614	CLA	CBA-CGA-O2A-C1
31	S1	617	CLA	CBA-CGA-O2A-C1
31	b1	608	CLA	CBA-CGA-O2A-C1
31	c1	506	CLA	CBA-CGA-O2A-C1
31	c1	509	CLA	CBA-CGA-O2A-C1
31	c1	511	CLA	CBA-CGA-O2A-C1
31	n1	602	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	g1	602	CLA	CBA-CGA-O2A-C1
31	g1	604	CLA	CBA-CGA-O2A-C1
31	r1	602	CLA	CBA-CGA-O2A-C1
31	r1	604	CLA	CBA-CGA-O2A-C1
31	r1	609	CLA	CBA-CGA-O2A-C1
31	s1	602	CLA	CBA-CGA-O2A-C1
31	s1	603	CLA	CBA-CGA-O2A-C1
31	s1	613	CLA	CBA-CGA-O2A-C1
31	y1	602	CLA	CBA-CGA-O2A-C1
31	y1	603	CLA	CBA-CGA-O2A-C1
31	y1	608	CLA	CBA-CGA-O2A-C1
34	M1	101	SQD	C24-C23-O48-C46
35	C1	523	LMG	C29-C28-O8-C9
35	c1	521	LMG	C29-C28-O8-C9
40	c1	520	DGD	C2A-C1A-O1G-C1G
52	S	626	3PH	C32-C31-O31-C3
52	i	101	3PH	C32-C31-O31-C3
52	T1	101	3PH	C32-C31-O31-C3
57	Y1	627	PTY	C31-C30-O4-C1
41	L1	101	LHG	C7-C8-C9-C10
35	d1	411	LMG	C20-C21-C22-C23
31	C	507	CLA	O1D-CGD-O2D-CED
31	N	602	CLA	O1D-CGD-O2D-CED
31	G	604	CLA	O1D-CGD-O2D-CED
31	S	604	CLA	O1D-CGD-O2D-CED
31	D1	403	CLA	O1D-CGD-O2D-CED
31	N1	611	CLA	O1D-CGD-O2D-CED
31	b1	613	CLA	O1D-CGD-O2D-CED
31	s1	605	CLA	O1D-CGD-O2D-CED
44	D	405	PL9	C47-C48-C49-C50
31	Y	604	CLA	CBD-CGD-O2D-CED
31	A	410	CLA	O1D-CGD-O2D-CED
31	B	607	CLA	O1D-CGD-O2D-CED
31	C	504	CLA	O1D-CGD-O2D-CED
31	R	604	CLA	O1D-CGD-O2D-CED
31	S	605	CLA	O1D-CGD-O2D-CED
31	S	610	CLA	O1D-CGD-O2D-CED
31	b	608	CLA	O1D-CGD-O2D-CED
31	b	613	CLA	O1D-CGD-O2D-CED
31	r	612	CLA	O1D-CGD-O2D-CED
31	s	613	CLA	O1D-CGD-O2D-CED
31	y	603	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	y	611	CLA	O1D-CGD-O2D-CED
31	C1	504	CLA	O1D-CGD-O2D-CED
31	a1	407	CLA	O1D-CGD-O2D-CED
31	c1	511	CLA	O1D-CGD-O2D-CED
31	n1	611	CLA	O1D-CGD-O2D-CED
31	g1	602	CLA	O1D-CGD-O2D-CED
31	g1	603	CLA	O1D-CGD-O2D-CED
31	s1	609	CLA	O1D-CGD-O2D-CED
31	y1	603	CLA	O1D-CGD-O2D-CED
32	a	409	PHO	O1D-CGD-O2D-CED
40	c	520	DGD	O1B-C1B-O2G-C2G
41	s	624	LHG	O9-C7-O7-C5
44	D	405	PL9	C12-C13-C14-C16
44	D	405	PL9	C42-C43-C44-C46
44	D1	405	PL9	C22-C23-C24-C26
44	D1	405	PL9	C37-C38-C39-C41
44	d1	405	PL9	C37-C38-C39-C41
31	B	611	CLA	O1A-CGA-O2A-C1
31	C	511	CLA	O1A-CGA-O2A-C1
31	C	512	CLA	O1A-CGA-O2A-C1
31	D	403	CLA	O1A-CGA-O2A-C1
31	R	603	CLA	O1A-CGA-O2A-C1
31	R	612	CLA	O1A-CGA-O2A-C1
31	Y	612	CLA	O1A-CGA-O2A-C1
31	Y	613	CLA	O1A-CGA-O2A-C1
31	b	602	CLA	O1A-CGA-O2A-C1
31	b	605	CLA	O1A-CGA-O2A-C1
31	c	511	CLA	O1A-CGA-O2A-C1
31	s	602	CLA	O1A-CGA-O2A-C1
31	s	609	CLA	O1A-CGA-O2A-C1
31	s	617	CLA	O1A-CGA-O2A-C1
31	y	612	CLA	O1A-CGA-O2A-C1
31	B1	603	CLA	O1A-CGA-O2A-C1
31	C1	506	CLA	O1A-CGA-O2A-C1
31	C1	509	CLA	O1A-CGA-O2A-C1
31	C1	511	CLA	O1A-CGA-O2A-C1
31	G1	613	CLA	O1A-CGA-O2A-C1
31	S1	602	CLA	O1A-CGA-O2A-C1
31	Y1	602	CLA	O1A-CGA-O2A-C1
31	Y1	608	CLA	O1A-CGA-O2A-C1
31	Y1	613	CLA	O1A-CGA-O2A-C1
31	b1	606	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c1	506	CLA	O1A-CGA-O2A-C1
31	c1	509	CLA	O1A-CGA-O2A-C1
31	n1	603	CLA	O1A-CGA-O2A-C1
31	g1	613	CLA	O1A-CGA-O2A-C1
31	r1	608	CLA	O1A-CGA-O2A-C1
31	r1	609	CLA	O1A-CGA-O2A-C1
31	s1	602	CLA	O1A-CGA-O2A-C1
31	s1	617	CLA	O1A-CGA-O2A-C1
31	y1	603	CLA	O1A-CGA-O2A-C1
52	T1	101	3PH	O32-C31-O31-C3
57	y1	626	PTY	O30-C30-O4-C1
31	g	602	CLA	O1D-CGD-O2D-CED
31	n1	602	CLA	O1D-CGD-O2D-CED
33	c	514	BCR	C9-C10-C11-C12
33	C1	515	BCR	C9-C10-C11-C12
33	C1	515	BCR	C19-C20-C21-C22
33	D1	404	BCR	C19-C20-C21-C22
33	b1	618	BCR	C9-C10-C11-C12
33	c1	514	BCR	C9-C10-C11-C12
33	c1	517	BCR	C9-C10-C11-C12
37	b1	620	C7Z	C29-C30-C31-C32
46	H	101	RRX	C19-C20-C21-C22
46	H	101	RRX	C13-C14-C15-C16
46	H	101	RRX	C9-C10-C11-C12
48	n	621	LUT	C33-C34-C35-C15
49	R	621	XAT	C13-C14-C15-C35
49	r	622	XAT	C13-C14-C15-C35
31	d	402	CLA	CBD-CGD-O2D-CED
31	B1	602	CLA	CBD-CGD-O2D-CED
31	c1	506	CLA	CBD-CGD-O2D-CED
31	b	611	CLA	O1D-CGD-O2D-CED
31	y	602	CLA	O1D-CGD-O2D-CED
31	G1	611	CLA	O1D-CGD-O2D-CED
31	Y1	603	CLA	O1D-CGD-O2D-CED
31	b1	603	CLA	O1D-CGD-O2D-CED
31	c1	507	CLA	O1D-CGD-O2D-CED
41	C	525	LHG	O2-C2-C3-O3
41	G	630	LHG	O2-C2-C3-O3
41	S	624	LHG	O2-C2-C3-O3
41	d	409	LHG	O2-C2-C3-O3
41	l	101	LHG	O2-C2-C3-O3
41	g	624	LHG	O2-C2-C3-O3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	y	624	LHG	O2-C2-C3-O3
41	C1	525	LHG	O2-C2-C3-O3
41	D1	409	LHG	O2-C2-C3-O3
41	L1	101	LHG	O2-C2-C3-O3
41	S1	624	LHG	O2-C2-C3-O3
41	Y1	624	LHG	O2-C2-C3-O3
41	d1	409	LHG	O2-C2-C3-O3
41	n1	624	LHG	O2-C2-C3-O3
41	g1	624	LHG	O2-C2-C3-O3
41	s1	624	LHG	O2-C2-C3-O3
51	s	625	LPX	O1-C3-C4-O5
51	S1	625	LPX	O1-C3-C4-O5
31	C	501	CLA	C3-C5-C6-C7
31	Y	603	CLA	C3-C5-C6-C7
31	y	610	CLA	C3-C5-C6-C7
31	Y1	611	CLA	C3-C5-C6-C7
31	r1	612	CLA	C3-C5-C6-C7
31	y1	614	CLA	C3-C5-C6-C7
31	B	605	CLA	CBA-CGA-O2A-C1
31	B	606	CLA	CBA-CGA-O2A-C1
31	C	506	CLA	CBA-CGA-O2A-C1
31	N	603	CLA	CBA-CGA-O2A-C1
31	S	602	CLA	CBA-CGA-O2A-C1
31	b	611	CLA	CBA-CGA-O2A-C1
31	s	609	CLA	CBA-CGA-O2A-C1
31	A1	407	CLA	CBA-CGA-O2A-C1
31	C1	504	CLA	CBA-CGA-O2A-C1
31	D1	403	CLA	CBA-CGA-O2A-C1
31	N1	610	CLA	CBA-CGA-O2A-C1
31	N1	611	CLA	CBA-CGA-O2A-C1
31	R1	608	CLA	CBA-CGA-O2A-C1
31	Y1	603	CLA	CBA-CGA-O2A-C1
31	Y1	608	CLA	CBA-CGA-O2A-C1
31	Y1	612	CLA	CBA-CGA-O2A-C1
31	a1	407	CLA	CBA-CGA-O2A-C1
31	a1	410	CLA	CBA-CGA-O2A-C1
31	b1	614	CLA	CBA-CGA-O2A-C1
31	n1	603	CLA	CBA-CGA-O2A-C1
31	s1	617	CLA	CBA-CGA-O2A-C1
35	j	101	LMG	C29-C28-O8-C9
38	c1	524	DGA	CA2-CA1-OG1-CG1
40	c	520	DGD	C2A-C1A-O1G-C1G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	A	410	CLA	O1A-CGA-O2A-C1
31	B	608	CLA	O1A-CGA-O2A-C1
31	G	604	CLA	O1A-CGA-O2A-C1
31	R	608	CLA	O1A-CGA-O2A-C1
31	R	609	CLA	O1A-CGA-O2A-C1
31	b	611	CLA	O1A-CGA-O2A-C1
31	r	612	CLA	O1A-CGA-O2A-C1
31	B1	613	CLA	O1A-CGA-O2A-C1
31	R1	609	CLA	O1A-CGA-O2A-C1
31	n1	602	CLA	O1A-CGA-O2A-C1
31	r1	602	CLA	O1A-CGA-O2A-C1
31	s1	613	CLA	O1A-CGA-O2A-C1
34	M1	101	SQD	O10-C23-O48-C46
35	d1	411	LMG	O6-C5-C6-O5
31	B	616	CLA	O1D-CGD-O2D-CED
31	C	509	CLA	O1D-CGD-O2D-CED
31	R	612	CLA	O1D-CGD-O2D-CED
31	b	603	CLA	O1D-CGD-O2D-CED
31	b1	609	CLA	O1D-CGD-O2D-CED
31	s1	602	CLA	O1D-CGD-O2D-CED
51	s	625	LPX	O5-C4-C5-O6
34	b1	626	SQD	C8-C7-O47-C45
35	B	622	LMG	C11-C10-O7-C8
38	b1	625	DGA	CB2-CB1-OG2-CG2
40	C	519	DGD	C2B-C1B-O2G-C2G
31	g	612	CLA	O1D-CGD-O2D-CED
31	Y	611	CLA	CBD-CGD-O2D-CED
55	r1	625	LMT	C4B-C5B-C6B-O6B
31	A1	407	CLA	O1A-CGA-O2A-C1
35	d	411	LMG	O6-C5-C6-O5
55	r1	625	LMT	O5'-C5'-C6'-O6'
31	B	603	CLA	O1D-CGD-O2D-CED
31	Y	603	CLA	O1D-CGD-O2D-CED
31	n	611	CLA	O1D-CGD-O2D-CED
31	a1	410	CLA	O1D-CGD-O2D-CED
31	y1	604	CLA	O1D-CGD-O2D-CED
31	B	612	CLA	CBD-CGD-O2D-CED
31	C	502	CLA	C3-C5-C6-C7
31	b	602	CLA	C3-C5-C6-C7
31	s	604	CLA	C3-C5-C6-C7
31	C1	509	CLA	C3-C5-C6-C7
31	a1	406	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s1	613	CLA	C3-C5-C6-C7
31	B	611	CLA	CBA-CGA-O2A-C1
31	c	510	CLA	CBA-CGA-O2A-C1
31	s	617	CLA	CBA-CGA-O2A-C1
31	B1	610	CLA	CBA-CGA-O2A-C1
31	N1	603	CLA	CBA-CGA-O2A-C1
31	Y1	613	CLA	CBA-CGA-O2A-C1
31	b1	603	CLA	CBA-CGA-O2A-C1
31	g1	613	CLA	CBA-CGA-O2A-C1
31	r1	608	CLA	CBA-CGA-O2A-C1
54	I1	102	4RF	C15-C16-O18-C19
31	Y	602	CLA	O1D-CGD-O2D-CED
31	B1	612	CLA	O1D-CGD-O2D-CED
38	b1	625	DGA	OB1-CB1-OG2-CG2
40	C	519	DGD	O1B-C1B-O2G-C2G
31	B	605	CLA	O1A-CGA-O2A-C1
31	B	606	CLA	O1A-CGA-O2A-C1
31	C	510	CLA	O1A-CGA-O2A-C1
31	r	608	CLA	O1A-CGA-O2A-C1
31	s	613	CLA	O1A-CGA-O2A-C1
31	y	614	CLA	O1A-CGA-O2A-C1
31	C1	504	CLA	O1A-CGA-O2A-C1
31	C1	513	CLA	O1A-CGA-O2A-C1
31	D1	403	CLA	O1A-CGA-O2A-C1
31	S1	614	CLA	O1A-CGA-O2A-C1
31	a1	407	CLA	O1A-CGA-O2A-C1
31	a1	410	CLA	O1A-CGA-O2A-C1
31	b1	608	CLA	O1A-CGA-O2A-C1
31	b1	614	CLA	O1A-CGA-O2A-C1
35	j	101	LMG	O10-C28-O8-C9
40	c1	520	DGD	O1A-C1A-O1G-C1G
45	F	101	HEM	C3D-CAD-CBD-CGD
45	F1	101	HEM	C3D-CAD-CBD-CGD
31	g	602	CLA	C4-C3-C5-C6
31	C1	504	CLA	C4-C3-C5-C6
31	N1	610	CLA	C4-C3-C5-C6
31	b1	604	CLA	C4-C3-C5-C6
31	b1	606	CLA	C4-C3-C5-C6
31	b1	615	CLA	C4-C3-C5-C6
47	n	601	CHL	C4-C3-C5-C6
31	C	513	CLA	C2-C3-C5-C6
31	c	501	CLA	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	d	402	CLA	C2-C3-C5-C6
31	g	602	CLA	C2-C3-C5-C6
31	C1	504	CLA	C2-C3-C5-C6
31	N1	610	CLA	C2-C3-C5-C6
31	b1	604	CLA	C2-C3-C5-C6
31	b1	606	CLA	C2-C3-C5-C6
31	b1	615	CLA	C2-C3-C5-C6
44	d1	405	PL9	C33-C34-C36-C37
47	G	601	CHL	C2-C3-C5-C6
47	n	601	CHL	C2-C3-C5-C6
31	R	602	CLA	C2A-CAA-CBA-CGA
31	n	611	CLA	C2A-CAA-CBA-CGA
31	g	614	CLA	C2A-CAA-CBA-CGA
31	s	617	CLA	C2A-CAA-CBA-CGA
31	B1	603	CLA	C2A-CAA-CBA-CGA
31	G1	614	CLA	C2A-CAA-CBA-CGA
31	y1	610	CLA	C2A-CAA-CBA-CGA
32	A1	409	PHO	C2A-CAA-CBA-CGA
47	G	605	CHL	C2A-CAA-CBA-CGA
31	B	613	CLA	O1D-CGD-O2D-CED
31	N	611	CLA	O1D-CGD-O2D-CED
31	G	602	CLA	O1D-CGD-O2D-CED
31	R	602	CLA	O1D-CGD-O2D-CED
31	s1	604	CLA	O1D-CGD-O2D-CED
40	C1	520	DGD	O6E-C5E-C6E-O5E
31	C	506	CLA	O1A-CGA-O2A-C1
31	N	603	CLA	O1A-CGA-O2A-C1
31	a	405	CLA	O1A-CGA-O2A-C1
31	b	608	CLA	O1A-CGA-O2A-C1
31	c	510	CLA	O1A-CGA-O2A-C1
31	r	603	CLA	O1A-CGA-O2A-C1
31	B1	610	CLA	O1A-CGA-O2A-C1
31	N1	610	CLA	O1A-CGA-O2A-C1
31	Y1	603	CLA	O1A-CGA-O2A-C1
31	Y1	612	CLA	O1A-CGA-O2A-C1
31	r1	604	CLA	O1A-CGA-O2A-C1
31	y1	602	CLA	O1A-CGA-O2A-C1
38	c1	524	DGA	OA1-CA1-OG1-CG1
40	c	519	DGD	O1A-C1A-O1G-C1G
44	D	405	PL9	C34-C36-C37-C38
44	D1	405	PL9	C19-C21-C22-C23
44	d1	405	PL9	C29-C31-C32-C33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N	602	CLA	C3-C5-C6-C7
31	b	614	CLA	C3-C5-C6-C7
31	b	606	CLA	CBA-CGA-O2A-C1
31	g	602	CLA	CBA-CGA-O2A-C1
31	r	604	CLA	CBA-CGA-O2A-C1
31	B1	608	CLA	CBA-CGA-O2A-C1
31	c1	508	CLA	CBA-CGA-O2A-C1
35	c1	523	LMG	C29-C28-O8-C9
40	c	519	DGD	C2A-C1A-O1G-C1G
41	L1	101	LHG	C24-C23-O8-C6
31	C	510	CLA	O1D-CGD-O2D-CED
31	S	612	CLA	O1D-CGD-O2D-CED
31	c	501	CLA	O1D-CGD-O2D-CED
31	c	507	CLA	O1D-CGD-O2D-CED
31	c	510	CLA	O1D-CGD-O2D-CED
31	C1	507	CLA	O1D-CGD-O2D-CED
31	S1	612	CLA	O1D-CGD-O2D-CED
31	Y1	602	CLA	O1D-CGD-O2D-CED
31	Y1	612	CLA	O1D-CGD-O2D-CED
31	n1	604	CLA	O1D-CGD-O2D-CED
31	R1	608	CLA	O1A-CGA-O2A-C1
40	c	520	DGD	O1A-C1A-O1G-C1G
34	m1	101	SQD	C8-C7-O47-C45
38	B1	625	DGA	CB2-CB1-OG2-CG2
44	D1	405	PL9	C47-C48-C49-C51
55	R1	625	LMT	C4B-C5B-C6B-O6B
44	d1	405	PL9	C22-C23-C24-C25
31	C	502	CLA	O1D-CGD-O2D-CED
31	C	513	CLA	O1D-CGD-O2D-CED
31	S	614	CLA	O1D-CGD-O2D-CED
31	b	609	CLA	O1D-CGD-O2D-CED
31	b	616	CLA	O1D-CGD-O2D-CED
31	s	605	CLA	O1D-CGD-O2D-CED
31	B1	609	CLA	O1D-CGD-O2D-CED
31	B1	613	CLA	O1D-CGD-O2D-CED
31	N1	604	CLA	O1D-CGD-O2D-CED
31	g1	612	CLA	O1D-CGD-O2D-CED
31	r1	602	CLA	O1D-CGD-O2D-CED
31	g	613	CLA	C8-C10-C11-C12
31	G1	612	CLA	O1D-CGD-O2D-CED
41	L	101	LHG	C1-C2-C3-O3
41	G	630	LHG	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	l	101	LHG	C1-C2-C3-O3
41	L1	101	LHG	C1-C2-C3-O3
41	G1	624	LHG	C1-C2-C3-O3
41	Y1	624	LHG	C1-C2-C3-O3
41	c1	525	LHG	C1-C2-C3-O3
41	g1	624	LHG	C1-C2-C3-O3
51	S	625	LPX	O1-C3-C4-C5
51	S1	625	LPX	O1-C3-C4-C5
34	m1	101	SQD	O49-C7-O47-C45
31	A	405	CLA	O1A-CGA-O2A-C1
31	b	606	CLA	O1A-CGA-O2A-C1
31	g	602	CLA	O1A-CGA-O2A-C1
31	r	604	CLA	O1A-CGA-O2A-C1
31	B1	608	CLA	O1A-CGA-O2A-C1
31	y1	610	CLA	O1A-CGA-O2A-C1
35	c1	523	LMG	O10-C28-O8-C9
41	L1	101	LHG	O10-C23-O8-C6
31	r	608	CLA	C3-C5-C6-C7
31	s	603	CLA	C3-C5-C6-C7
31	y	613	CLA	C3-C5-C6-C7
31	B1	603	CLA	C3-C5-C6-C7
31	c1	511	CLA	C3-C5-C6-C7
31	N	610	CLA	O1D-CGD-O2D-CED
31	c	513	CLA	O1D-CGD-O2D-CED
31	y	614	CLA	O1D-CGD-O2D-CED
31	S1	602	CLA	O1D-CGD-O2D-CED
31	A	405	CLA	CBA-CGA-O2A-C1
31	B	612	CLA	CBA-CGA-O2A-C1
31	B	614	CLA	CBA-CGA-O2A-C1
31	C	509	CLA	CBA-CGA-O2A-C1
31	G	603	CLA	CBA-CGA-O2A-C1
31	S	604	CLA	CBA-CGA-O2A-C1
31	Y	614	CLA	CBA-CGA-O2A-C1
31	a	410	CLA	CBA-CGA-O2A-C1
31	b	604	CLA	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	b	614	CLA	CBA-CGA-O2A-C1
31	c	503	CLA	CBA-CGA-O2A-C1
31	c	506	CLA	CBA-CGA-O2A-C1
31	c	507	CLA	CBA-CGA-O2A-C1
31	n	611	CLA	CBA-CGA-O2A-C1
31	g	603	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s	611	CLA	CBA-CGA-O2A-C1
31	B1	602	CLA	CBA-CGA-O2A-C1
31	B1	604	CLA	CBA-CGA-O2A-C1
31	B1	614	CLA	CBA-CGA-O2A-C1
31	B1	617	CLA	CBA-CGA-O2A-C1
31	N1	602	CLA	CBA-CGA-O2A-C1
31	R1	602	CLA	CBA-CGA-O2A-C1
31	R1	604	CLA	CBA-CGA-O2A-C1
31	a1	405	CLA	CBA-CGA-O2A-C1
31	b1	604	CLA	CBA-CGA-O2A-C1
31	b1	613	CLA	CBA-CGA-O2A-C1
31	y1	610	CLA	CBA-CGA-O2A-C1
34	b	621	SQD	C24-C23-O48-C46
34	m1	101	SQD	C24-C23-O48-C46
35	B1	622	LMG	C29-C28-O8-C9
40	C	519	DGD	C2A-C1A-O1G-C1G
40	C	520	DGD	C2A-C1A-O1G-C1G
40	c	518	DGD	C2A-C1A-O1G-C1G
40	C1	518	DGD	C2A-C1A-O1G-C1G
41	c1	525	LHG	C24-C23-O8-C6
52	S1	626	3PH	C32-C31-O31-C3
55	R1	625	LMT	O5'-C5'-C6'-O6'
31	s1	603	CLA	O1D-CGD-O2D-CED
33	c1	515	BCR	C9-C10-C11-C12
46	h	101	RRX	C19-C20-C21-C22
48	Y	621	LUT	C29-C30-C31-C32
41	s	624	LHG	C7-C8-C9-C10
31	d	402	CLA	C15-C16-C17-C18
31	B1	603	CLA	C10-C11-C12-C13
31	B1	604	CLA	C10-C11-C12-C13
31	B1	608	CLA	C10-C11-C12-C13
31	s1	610	CLA	C8-C10-C11-C12
31	B1	614	CLA	O1A-CGA-O2A-C1
31	B	611	CLA	C15-C16-C17-C18
31	N	602	CLA	C5-C6-C7-C8
31	G	602	CLA	C13-C15-C16-C17
31	S	613	CLA	C5-C6-C7-C8
31	a	410	CLA	C8-C10-C11-C12
31	b	603	CLA	C10-C11-C12-C13
31	y	604	CLA	C15-C16-C17-C18
31	B1	609	CLA	C5-C6-C7-C8
31	N1	602	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N1	602	CLA	C10-C11-C12-C13
31	G1	603	CLA	C15-C16-C17-C18
31	b1	602	CLA	C8-C10-C11-C12
31	d1	403	CLA	C8-C10-C11-C12
31	s1	604	CLA	C5-C6-C7-C8
41	D	409	LHG	O2-C2-C3-O3
41	L	101	LHG	O2-C2-C3-O3
41	c1	525	LHG	O2-C2-C3-O3
31	C	507	CLA	C3-C5-C6-C7
38	B	625	DGA	CA1-CA2-CA3-CA4
38	C	524	DGA	CB1-CB2-CB3-CB4
34	C	526	SQD	C2-C1-O6-C44
34	c	626	SQD	C2-C1-O6-C44
34	a1	412	SQD	C2-C1-O6-C44
34	c1	526	SQD	C2-C1-O6-C44
40	C	519	DGD	C2D-C1D-O3G-C3G
40	c	519	DGD	C2D-C1D-O3G-C3G
35	a	413	LMG	O1-C7-C8-O7
41	g	624	LHG	O7-C5-C6-O8
52	S1	626	3PH	C32-C33-C34-C35
31	Y	614	CLA	O1A-CGA-O2A-C1
31	b	613	CLA	O1A-CGA-O2A-C1
31	c	503	CLA	O1A-CGA-O2A-C1
31	g	603	CLA	O1A-CGA-O2A-C1
34	b	621	SQD	O10-C23-O48-C46
40	C1	518	DGD	O1A-C1A-O1G-C1G
35	a1	413	LMG	O6-C5-C6-O5
40	c1	520	DGD	O6E-C5E-C6E-O5E
31	c	503	CLA	C2-C3-C5-C6
31	C1	503	CLA	C2-C3-C5-C6
31	C1	505	CLA	C2-C3-C5-C6
31	c1	504	CLA	C2-C3-C5-C6
31	r1	610	CLA	C2-C3-C5-C6
47	G	609	CHL	C2-C3-C5-C6
47	Y	606	CHL	C2-C3-C5-C6
31	B	612	CLA	C11-C12-C13-C14
31	B	616	CLA	C6-C7-C8-C9
31	C	501	CLA	C11-C12-C13-C14
31	C	506	CLA	C11-C12-C13-C14
31	C	507	CLA	C11-C10-C8-C9
31	D	402	CLA	C6-C7-C8-C9
31	G	602	CLA	C14-C13-C15-C16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	603	CLA	C11-C10-C8-C9
31	Y	602	CLA	C14-C13-C15-C16
31	b	604	CLA	C14-C13-C15-C16
31	c	502	CLA	C6-C7-C8-C9
31	c	507	CLA	C11-C10-C8-C9
31	c	513	CLA	C11-C10-C8-C9
31	d	402	CLA	C6-C7-C8-C9
31	r	603	CLA	C11-C10-C8-C9
31	r	610	CLA	C11-C10-C8-C9
31	y	602	CLA	C11-C10-C8-C9
31	D1	402	CLA	C6-C7-C8-C9
31	R1	602	CLA	C6-C7-C8-C9
31	R1	610	CLA	C6-C7-C8-C9
31	R1	612	CLA	C6-C7-C8-C9
31	Y1	604	CLA	C11-C10-C8-C9
31	a1	406	CLA	C14-C13-C15-C16
31	b1	605	CLA	C6-C7-C8-C9
31	b1	607	CLA	C14-C13-C15-C16
31	b1	612	CLA	C11-C12-C13-C14
31	b1	617	CLA	C14-C13-C15-C16
31	c1	505	CLA	C6-C7-C8-C9
31	c1	511	CLA	C6-C7-C8-C9
31	c1	513	CLA	C11-C10-C8-C9
31	d1	402	CLA	C6-C7-C8-C9
31	n1	613	CLA	C14-C13-C15-C16
31	r1	608	CLA	C11-C10-C8-C9
31	r1	612	CLA	C6-C7-C8-C9
31	s1	609	CLA	C11-C10-C8-C9
31	y1	604	CLA	C6-C7-C8-C9
31	y1	611	CLA	C11-C12-C13-C14
32	A	409	PHO	C6-C7-C8-C9
32	a	409	PHO	C6-C7-C8-C9
32	a1	409	PHO	C6-C7-C8-C9
47	Y	601	CHL	C11-C10-C8-C9
47	Y	607	CHL	C11-C10-C8-C9
47	Y	607	CHL	C14-C13-C15-C16
47	n	605	CHL	C11-C10-C8-C9
47	g	609	CHL	C11-C10-C8-C9
47	y	601	CHL	C11-C10-C8-C9
47	N1	606	CHL	C14-C13-C15-C16
47	G1	601	CHL	C14-C13-C15-C16
47	G1	607	CHL	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	Y1	607	CHL	C14-C13-C15-C16
47	Y1	609	CHL	C11-C12-C13-C14
47	n1	606	CHL	C14-C13-C15-C16
47	n1	607	CHL	C14-C13-C15-C16
47	g1	601	CHL	C14-C13-C15-C16
47	y1	609	CHL	C11-C12-C13-C14
31	N	603	CLA	O1D-CGD-O2D-CED
31	a	410	CLA	O1D-CGD-O2D-CED
31	r	610	CLA	O1D-CGD-O2D-CED
31	y	612	CLA	O1D-CGD-O2D-CED
31	A1	410	CLA	O1D-CGD-O2D-CED
31	n1	603	CLA	O1D-CGD-O2D-CED
41	y	624	LHG	C33-C34-C35-C36
31	B	603	CLA	C5-C6-C7-C8
31	B	613	CLA	C5-C6-C7-C8
31	b	602	CLA	C15-C16-C17-C18
31	B1	604	CLA	C8-C10-C11-C12
31	B1	604	CLA	C15-C16-C17-C18
31	g1	611	CLA	C15-C16-C17-C18
31	S	613	CLA	C2A-CAA-CBA-CGA
31	g	604	CLA	C2A-CAA-CBA-CGA
31	Y1	602	CLA	C2A-CAA-CBA-CGA
31	c1	502	CLA	C2A-CAA-CBA-CGA
31	g1	602	CLA	C2A-CAA-CBA-CGA
31	y1	602	CLA	C2A-CAA-CBA-CGA
47	n	606	CHL	C2A-CAA-CBA-CGA
33	B	619	BCR	C37-C22-C23-C24
33	C	514	BCR	C11-C12-C13-C35
33	C	515	BCR	C37-C22-C23-C24
33	b	619	BCR	C11-C12-C13-C35
33	c	515	BCR	C7-C8-C9-C34
33	B1	618	BCR	C37-C22-C23-C24
33	C1	514	BCR	C36-C18-C19-C20
33	C1	515	BCR	C7-C8-C9-C34
33	C1	515	BCR	C36-C18-C19-C20
33	C1	517	BCR	C7-C8-C9-C34
33	C1	517	BCR	C37-C22-C23-C24
33	a1	411	BCR	C7-C8-C9-C34
33	c1	515	BCR	C11-C12-C13-C35
33	c1	516	BCR	C7-C8-C9-C34
37	B	620	C7Z	C31-C32-C33-C40
37	b	620	C7Z	C31-C32-C33-C40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
37	B1	620	C7Z	C7-C8-C9-C19
37	b1	620	C7Z	C7-C8-C9-C19
46	h	101	RRX	C36-C18-C19-C20
46	H1	101	RRX	C7-C8-C9-C34
48	R	620	LUT	C7-C8-C9-C19
48	r	620	LUT	C7-C8-C9-C19
49	Y	622	XAT	C27-C28-C29-C39
49	y	622	XAT	C11-C12-C13-C20
49	n1	622	XAT	C31-C32-C33-C40
50	s	623	NEX	C11-C12-C13-C20
33	B	619	BCR	C21-C22-C23-C24
33	b	618	BCR	C7-C8-C9-C10
33	c	517	BCR	C17-C18-C19-C20
33	C1	515	BCR	C7-C8-C9-C10
33	C1	517	BCR	C21-C22-C23-C24
33	c1	516	BCR	C7-C8-C9-C10
37	B	620	C7Z	C31-C32-C33-C34
37	b	620	C7Z	C31-C32-C33-C34
37	B1	620	C7Z	C7-C8-C9-C10
37	b1	620	C7Z	C7-C8-C9-C10
46	H1	101	RRX	C7-C8-C9-C10
48	R	620	LUT	C7-C8-C9-C10
48	r	620	LUT	C7-C8-C9-C10
31	N1	612	CLA	O1D-CGD-O2D-CED
34	B1	621	SQD	C8-C7-O47-C45
38	c	524	DGA	CB2-CB1-OG2-CG2
40	c	519	DGD	C2B-C1B-O2G-C2G
40	C1	520	DGD	C4E-C5E-C6E-O5E
34	B1	621	SQD	C23-C24-C25-C26
35	b	622	LMG	C10-C11-C12-C13
35	h	102	LMG	C28-C29-C30-C31
41	C	525	LHG	C23-C24-C25-C26
41	Y	624	LHG	C7-C8-C9-C10
41	c	625	LHG	C23-C24-C25-C26
57	y1	626	PTY	C8-C11-C12-C13
31	C	509	CLA	O1A-CGA-O2A-C1
31	a	410	CLA	O1A-CGA-O2A-C1
31	c	506	CLA	O1A-CGA-O2A-C1
31	n	611	CLA	O1A-CGA-O2A-C1
31	B1	617	CLA	O1A-CGA-O2A-C1
31	R1	604	CLA	O1A-CGA-O2A-C1
31	B	614	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B	614	CLA	C8-C10-C11-C12
31	C	502	CLA	C5-C6-C7-C8
31	R	612	CLA	C10-C11-C12-C13
31	S	611	CLA	C15-C16-C17-C18
31	c	506	CLA	C5-C6-C7-C8
31	d	403	CLA	C10-C11-C12-C13
31	B1	617	CLA	C8-C10-C11-C12
31	D1	402	CLA	C15-C16-C17-C18
31	S1	604	CLA	C5-C6-C7-C8
31	Y1	602	CLA	C13-C15-C16-C17
31	Y1	610	CLA	C15-C16-C17-C18
31	Y1	613	CLA	C5-C6-C7-C8
31	b1	605	CLA	C5-C6-C7-C8
31	b1	608	CLA	C13-C15-C16-C17
31	c1	510	CLA	C15-C16-C17-C18
31	s1	609	CLA	C5-C6-C7-C8
31	s1	611	CLA	C8-C10-C11-C12
31	y1	604	CLA	C8-C10-C11-C12
31	y1	610	CLA	C5-C6-C7-C8
31	C	506	CLA	O1D-CGD-O2D-CED
31	R1	602	CLA	O1D-CGD-O2D-CED
31	d1	402	CLA	O1D-CGD-O2D-CED
41	C1	525	LHG	C33-C34-C35-C36
41	S1	624	LHG	C26-C27-C28-C29
41	d1	410	LHG	C29-C30-C31-C32
54	k1	101	4RF	C46-C47-C48-C49
41	L	101	LHG	C11-C10-C9-C8
41	l	101	LHG	C11-C10-C9-C8
31	B	614	CLA	C3-C5-C6-C7
31	C	511	CLA	C3-C5-C6-C7
47	g1	601	CHL	C3-C5-C6-C7
31	B	602	CLA	CBA-CGA-O2A-C1
31	b	612	CLA	CBA-CGA-O2A-C1
31	c1	504	CLA	CBA-CGA-O2A-C1
38	b	623	DGA	CA2-CA1-OG1-CG1
31	B	604	CLA	C13-C15-C16-C17
31	B	608	CLA	C13-C15-C16-C17
31	B	609	CLA	C8-C10-C11-C12
31	B	617	CLA	C5-C6-C7-C8
31	C	502	CLA	C8-C10-C11-C12
31	C	507	CLA	C5-C6-C7-C8
31	C	507	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N	602	CLA	C15-C16-C17-C18
31	N	603	CLA	C10-C11-C12-C13
31	N	604	CLA	C13-C15-C16-C17
31	Y	613	CLA	C8-C10-C11-C12
31	b	603	CLA	C13-C15-C16-C17
31	b	605	CLA	C15-C16-C17-C18
31	b	607	CLA	C10-C11-C12-C13
31	b	613	CLA	C10-C11-C12-C13
31	c	501	CLA	C5-C6-C7-C8
31	c	503	CLA	C10-C11-C12-C13
31	c	503	CLA	C15-C16-C17-C18
31	c	507	CLA	C15-C16-C17-C18
31	n	602	CLA	C5-C6-C7-C8
31	n	604	CLA	C10-C11-C12-C13
31	g	603	CLA	C5-C6-C7-C8
31	y	603	CLA	C15-C16-C17-C18
31	y	611	CLA	C8-C10-C11-C12
31	y	611	CLA	C10-C11-C12-C13
31	y	614	CLA	C10-C11-C12-C13
31	y	614	CLA	C13-C15-C16-C17
31	A1	406	CLA	C15-C16-C17-C18
31	B1	608	CLA	C5-C6-C7-C8
31	B1	610	CLA	C5-C6-C7-C8
31	B1	610	CLA	C15-C16-C17-C18
31	B1	616	CLA	C8-C10-C11-C12
31	C1	513	CLA	C8-C10-C11-C12
31	N1	602	CLA	C13-C15-C16-C17
31	G1	602	CLA	C8-C10-C11-C12
31	G1	611	CLA	C15-C16-C17-C18
31	R1	608	CLA	C5-C6-C7-C8
31	S1	611	CLA	C5-C6-C7-C8
31	S1	611	CLA	C8-C10-C11-C12
31	Y1	611	CLA	C10-C11-C12-C13
31	Y1	612	CLA	C13-C15-C16-C17
31	b1	616	CLA	C13-C15-C16-C17
31	c1	503	CLA	C5-C6-C7-C8
31	c1	503	CLA	C8-C10-C11-C12
31	c1	503	CLA	C15-C16-C17-C18
31	c1	508	CLA	C5-C6-C7-C8
31	g1	603	CLA	C13-C15-C16-C17
31	g1	603	CLA	C15-C16-C17-C18
31	r1	608	CLA	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s1	602	CLA	C10-C11-C12-C13
31	s1	610	CLA	C10-C11-C12-C13
47	N1	606	CHL	C5-C6-C7-C8
40	C1	518	DGD	O6E-C5E-C6E-O5E
35	A1	413	LMG	C10-C11-C12-C13
35	H1	102	LMG	C28-C29-C30-C31
38	j1	101	DGA	CA1-CA2-CA3-CA4
40	B1	623	DGD	C1B-C2B-C3B-C4B
41	C	525	LHG	C7-C8-C9-C10
41	D	408	LHG	C7-C8-C9-C10
54	I1	102	4RF	C13-C14-C15-C16
40	C	519	DGD	O1A-C1A-O1G-C1G
56	R1	626	ERG	C17-C20-C22-C23
56	r1	626	ERG	C17-C20-C22-C23
31	A	410	CLA	C10-C11-C12-C13
31	B	604	CLA	C5-C6-C7-C8
31	B	607	CLA	C10-C11-C12-C13
31	B	608	CLA	C8-C10-C11-C12
31	B	612	CLA	C8-C10-C11-C12
31	B	612	CLA	C15-C16-C17-C18
31	B	615	CLA	C8-C10-C11-C12
31	R	609	CLA	C5-C6-C7-C8
31	R	612	CLA	C8-C10-C11-C12
31	Y	610	CLA	C15-C16-C17-C18
31	Y	611	CLA	C5-C6-C7-C8
31	b	604	CLA	C5-C6-C7-C8
31	b	604	CLA	C8-C10-C11-C12
31	b	608	CLA	C5-C6-C7-C8
31	b	611	CLA	C15-C16-C17-C18
31	b	614	CLA	C5-C6-C7-C8
31	c	502	CLA	C8-C10-C11-C12
31	c	505	CLA	C13-C15-C16-C17
31	c	507	CLA	C5-C6-C7-C8
31	c	513	CLA	C10-C11-C12-C13
31	g	602	CLA	C13-C15-C16-C17
31	g	603	CLA	C8-C10-C11-C12
31	g	610	CLA	C8-C10-C11-C12
31	y	602	CLA	C10-C11-C12-C13
31	B1	602	CLA	C13-C15-C16-C17
31	B1	606	CLA	C5-C6-C7-C8
31	B1	608	CLA	C13-C15-C16-C17
31	B1	611	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N1	603	CLA	C13-C15-C16-C17
31	N1	613	CLA	C8-C10-C11-C12
31	G1	603	CLA	C8-C10-C11-C12
31	R1	603	CLA	C10-C11-C12-C13
31	S1	602	CLA	C10-C11-C12-C13
31	S1	610	CLA	C5-C6-C7-C8
31	S1	610	CLA	C10-C11-C12-C13
31	Y1	611	CLA	C5-C6-C7-C8
31	Y1	614	CLA	C5-C6-C7-C8
31	a1	406	CLA	C5-C6-C7-C8
31	a1	410	CLA	C5-C6-C7-C8
31	b1	602	CLA	C10-C11-C12-C13
31	b1	608	CLA	C8-C10-C11-C12
31	b1	611	CLA	C15-C16-C17-C18
31	b1	612	CLA	C13-C15-C16-C17
31	c1	508	CLA	C13-C15-C16-C17
31	c1	513	CLA	C8-C10-C11-C12
31	n1	603	CLA	C5-C6-C7-C8
31	g1	602	CLA	C10-C11-C12-C13
31	g1	613	CLA	C15-C16-C17-C18
31	r1	608	CLA	C8-C10-C11-C12
31	r1	610	CLA	C5-C6-C7-C8
31	s1	609	CLA	C8-C10-C11-C12
31	s1	609	CLA	C10-C11-C12-C13
31	s1	611	CLA	C13-C15-C16-C17
31	y1	603	CLA	C10-C11-C12-C13
31	y1	604	CLA	C5-C6-C7-C8
31	y1	604	CLA	C15-C16-C17-C18
31	y1	611	CLA	C5-C6-C7-C8
31	y1	612	CLA	C10-C11-C12-C13
31	y1	613	CLA	C8-C10-C11-C12
31	C	501	CLA	O1D-CGD-O2D-CED
41	c	625	LHG	O1-C1-C2-O2
41	d	408	LHG	O1-C1-C2-O2
41	g1	624	LHG	O1-C1-C2-O2
34	M1	101	SQD	C7-C8-C9-C10
34	b1	621	SQD	C23-C24-C25-C26
34	m1	101	SQD	C7-C8-C9-C10
35	a	413	LMG	C28-C29-C30-C31
38	c	524	DGA	CB1-CB2-CB3-CB4
38	J1	101	DGA	CB1-CB2-CB3-CB4
38	b1	625	DGA	CB1-CB2-CB3-CB4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
40	c	520	DGD	C1A-C2A-C3A-C4A
40	c1	518	DGD	C1B-C2B-C3B-C4B
41	L	101	LHG	C7-C8-C9-C10
41	c	625	LHG	C7-C8-C9-C10
41	d	408	LHG	C7-C8-C9-C10
41	C1	525	LHG	C23-C24-C25-C26
41	D1	410	LHG	C23-C24-C25-C26
41	N1	624	LHG	C7-C8-C9-C10
41	G1	624	LHG	C7-C8-C9-C10
41	c1	525	LHG	C23-C24-C25-C26
41	d1	408	LHG	C23-C24-C25-C26
41	d1	409	LHG	C7-C8-C9-C10
41	d1	410	LHG	C23-C24-C25-C26
41	n1	624	LHG	C7-C8-C9-C10
52	b1	624	3PH	C31-C32-C33-C34
52	s1	626	3PH	C31-C32-C33-C34
54	K1	101	4RF	C41-C43-C44-C45
54	i1	101	4RF	C41-C43-C44-C45
35	H	102	LMG	O6-C5-C6-O5
31	B	613	CLA	C13-C15-C16-C17
31	C	502	CLA	C15-C16-C17-C18
31	C	503	CLA	C15-C16-C17-C18
31	C	506	CLA	C5-C6-C7-C8
31	G	603	CLA	C15-C16-C17-C18
31	b	603	CLA	C8-C10-C11-C12
31	c	506	CLA	C8-C10-C11-C12
31	n	610	CLA	C15-C16-C17-C18
31	g	603	CLA	C10-C11-C12-C13
31	g	613	CLA	C15-C16-C17-C18
31	r	608	CLA	C5-C6-C7-C8
31	r	608	CLA	C10-C11-C12-C13
31	y	610	CLA	C13-C15-C16-C17
31	y	614	CLA	C15-C16-C17-C18
31	B1	615	CLA	C5-C6-C7-C8
31	B1	616	CLA	C13-C15-C16-C17
31	C1	504	CLA	C10-C11-C12-C13
31	G1	611	CLA	C10-C11-C12-C13
31	G1	611	CLA	C13-C15-C16-C17
31	R1	603	CLA	C5-C6-C7-C8
31	S1	603	CLA	C13-C15-C16-C17
31	a1	406	CLA	C15-C16-C17-C18
31	b1	604	CLA	C10-C11-C12-C13

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
31	b1	610	CLA	C5-C6-C7-C8
31	c1	509	CLA	C15-C16-C17-C18
31	n1	604	CLA	C8-C10-C11-C12
31	y1	613	CLA	C15-C16-C17-C18
31	a	410	CLA	C3-C5-C6-C7
31	N1	610	CLA	C3-C5-C6-C7
31	C1	503	CLA	CBA-CGA-O2A-C1
40	C	518	DGD	C2A-C1A-O1G-C1G
31	c	506	CLA	O1D-CGD-O2D-CED
34	B1	621	SQD	O49-C7-O47-C45
34	b1	626	SQD	O49-C7-O47-C45
38	B1	625	DGA	OB1-CB1-OG2-CG2
31	A	406	CLA	C2-C1-O2A-CGA
31	B	602	CLA	C2-C1-O2A-CGA
31	B	613	CLA	C2-C1-O2A-CGA
31	C	506	CLA	C2-C1-O2A-CGA
31	C	509	CLA	C2-C1-O2A-CGA
31	C	512	CLA	C2-C1-O2A-CGA
31	N	603	CLA	C2-C1-O2A-CGA
31	N	611	CLA	C2-C1-O2A-CGA
31	G	614	CLA	C2-C1-O2A-CGA
31	R	609	CLA	C2-C1-O2A-CGA
31	Y	603	CLA	C2-C1-O2A-CGA
31	Y	608	CLA	C2-C1-O2A-CGA
31	Y	614	CLA	C2-C1-O2A-CGA
31	a	406	CLA	C2-C1-O2A-CGA
31	b	602	CLA	C2-C1-O2A-CGA
31	b	608	CLA	C2-C1-O2A-CGA
31	b	612	CLA	C2-C1-O2A-CGA
31	b	613	CLA	C2-C1-O2A-CGA
31	b	614	CLA	C2-C1-O2A-CGA
31	c	506	CLA	C2-C1-O2A-CGA
31	c	509	CLA	C2-C1-O2A-CGA
31	n	613	CLA	C2-C1-O2A-CGA
31	g	602	CLA	C2-C1-O2A-CGA
31	r	609	CLA	C2-C1-O2A-CGA
31	s	610	CLA	C2-C1-O2A-CGA
31	y	604	CLA	C2-C1-O2A-CGA
31	B1	603	CLA	C2-C1-O2A-CGA
31	B1	608	CLA	C2-C1-O2A-CGA
31	C1	502	CLA	C2-C1-O2A-CGA
31	C1	503	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C1	510	CLA	C2-C1-O2A-CGA
31	N1	603	CLA	C2-C1-O2A-CGA
31	N1	613	CLA	C2-C1-O2A-CGA
31	G1	604	CLA	C2-C1-O2A-CGA
31	Y1	603	CLA	C2-C1-O2A-CGA
31	Y1	604	CLA	C2-C1-O2A-CGA
31	Y1	608	CLA	C2-C1-O2A-CGA
31	Y1	614	CLA	C2-C1-O2A-CGA
31	a1	406	CLA	C2-C1-O2A-CGA
31	a1	407	CLA	C2-C1-O2A-CGA
31	c1	502	CLA	C2-C1-O2A-CGA
31	c1	509	CLA	C2-C1-O2A-CGA
31	n1	611	CLA	C2-C1-O2A-CGA
31	r1	603	CLA	C2-C1-O2A-CGA
31	r1	608	CLA	C2-C1-O2A-CGA
31	y1	603	CLA	C2-C1-O2A-CGA
31	y1	608	CLA	C2-C1-O2A-CGA
31	B	602	CLA	C10-C11-C12-C13
31	B	612	CLA	C10-C11-C12-C13
31	D	403	CLA	C15-C16-C17-C18
31	N	613	CLA	C8-C10-C11-C12
31	Y	610	CLA	C5-C6-C7-C8
31	Y	614	CLA	C8-C10-C11-C12
31	b	613	CLA	C15-C16-C17-C18
31	n	610	CLA	C5-C6-C7-C8
31	r	608	CLA	C8-C10-C11-C12
31	s	603	CLA	C15-C16-C17-C18
31	N1	604	CLA	C10-C11-C12-C13
31	N1	613	CLA	C5-C6-C7-C8
31	G1	613	CLA	C13-C15-C16-C17
31	Y1	604	CLA	C13-C15-C16-C17
31	g1	602	CLA	C13-C15-C16-C17
31	r1	609	CLA	C5-C6-C7-C8
31	A1	407	CLA	O1D-CGD-O2D-CED
34	b	621	SQD	C23-C24-C25-C26
35	C	521	LMG	C10-C11-C12-C13
41	D	408	LHG	C23-C24-C25-C26
41	D	410	LHG	C23-C24-C25-C26
41	G	630	LHG	C23-C24-C25-C26
41	S	624	LHG	C23-C24-C25-C26
41	n	624	LHG	C7-C8-C9-C10
41	D1	408	LHG	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	L1	101	LHG	C23-C24-C25-C26
41	c1	525	LHG	C7-C8-C9-C10
41	d1	409	LHG	C23-C24-C25-C26
41	g1	624	LHG	C7-C8-C9-C10
41	s1	624	LHG	C23-C24-C25-C26
31	b1	605	CLA	CBD-CGD-O2D-CED
35	h1	102	LMG	C15-C16-C17-C18
54	k1	101	4RF	C48-C49-C50-C51
41	g	624	LHG	C8-C7-O7-C5
57	Y1	626	PTY	C11-C8-O7-C6
31	A	410	CLA	C5-C6-C7-C8
31	B	607	CLA	C8-C10-C11-C12
31	R	602	CLA	C8-C10-C11-C12
31	b	617	CLA	C15-C16-C17-C18
31	g	610	CLA	C5-C6-C7-C8
31	g	613	CLA	C10-C11-C12-C13
31	y	604	CLA	C8-C10-C11-C12
31	A1	405	CLA	C5-C6-C7-C8
31	B1	603	CLA	C5-C6-C7-C8
31	B1	614	CLA	C8-C10-C11-C12
31	r1	602	CLA	C8-C10-C11-C12
31	s1	611	CLA	C15-C16-C17-C18
31	B	609	CLA	O1D-CGD-O2D-CED
31	B	604	CLA	C6-C7-C8-C10
31	G	610	CLA	C11-C12-C13-C15
31	R	603	CLA	C11-C10-C8-C7
31	Y	613	CLA	C11-C12-C13-C15
31	c	506	CLA	C6-C7-C8-C10
31	c	509	CLA	C11-C10-C8-C7
31	y	604	CLA	C11-C12-C13-C15
31	B1	602	CLA	C11-C10-C8-C7
31	C1	513	CLA	C6-C7-C8-C10
31	D1	403	CLA	C11-C10-C8-C7
31	R1	610	CLA	C6-C7-C8-C10
31	b1	617	CLA	C6-C7-C8-C10
31	c1	513	CLA	C6-C7-C8-C10
31	c1	513	CLA	C11-C12-C13-C15
31	n1	613	CLA	C12-C13-C15-C16
31	g1	603	CLA	C11-C12-C13-C15
31	r1	610	CLA	C11-C10-C8-C7
47	G	609	CHL	C11-C12-C13-C15
47	G1	601	CHL	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	n1	605	CHL	C11-C10-C8-C7
47	y1	609	CHL	C11-C12-C13-C15
31	B	602	CLA	O1A-CGA-O2A-C1
31	B	612	CLA	O1A-CGA-O2A-C1
31	b	614	CLA	O1A-CGA-O2A-C1
31	s	611	CLA	O1A-CGA-O2A-C1
31	B1	604	CLA	O1A-CGA-O2A-C1
31	N1	602	CLA	O1A-CGA-O2A-C1
34	m1	101	SQD	O10-C23-O48-C46
35	B1	622	LMG	O10-C28-O8-C9
40	c	518	DGD	O1A-C1A-O1G-C1G
33	A	411	BCR	C9-C10-C11-C12
33	C	517	BCR	C9-C10-C11-C12
33	c	516	BCR	C19-C20-C21-C22
33	B1	619	BCR	C19-C20-C21-C22
46	h	101	RRX	C9-C10-C11-C12
46	H1	101	RRX	C9-C10-C11-C12
46	h1	101	RRX	C15-C16-C17-C18
48	G	621	LUT	C33-C34-C35-C15
31	B	605	CLA	C2A-CAA-CBA-CGA
31	N	612	CLA	C2A-CAA-CBA-CGA
31	R	612	CLA	C2A-CAA-CBA-CGA
31	S	609	CLA	C2A-CAA-CBA-CGA
31	b	605	CLA	C2A-CAA-CBA-CGA
31	b	617	CLA	C2A-CAA-CBA-CGA
31	n	604	CLA	C2A-CAA-CBA-CGA
31	y	610	CLA	C2A-CAA-CBA-CGA
31	R1	602	CLA	C2A-CAA-CBA-CGA
31	b1	611	CLA	C2A-CAA-CBA-CGA
31	n1	604	CLA	C2A-CAA-CBA-CGA
31	s1	609	CLA	C2A-CAA-CBA-CGA
47	y	607	CHL	C2A-CAA-CBA-CGA
47	S1	608	CHL	C2A-CAA-CBA-CGA
47	Y1	606	CHL	C2A-CAA-CBA-CGA
31	B	614	CLA	C15-C16-C17-C18
31	B	616	CLA	C15-C16-C17-C18
31	B	617	CLA	C13-C15-C16-C17
31	C	513	CLA	C8-C10-C11-C12
31	N	604	CLA	C10-C11-C12-C13
31	R	602	CLA	C10-C11-C12-C13
31	Y	610	CLA	C13-C15-C16-C17
31	Y	614	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	Y	614	CLA	C10-C11-C12-C13
31	b	602	CLA	C10-C11-C12-C13
31	b	614	CLA	C10-C11-C12-C13
31	b	615	CLA	C8-C10-C11-C12
31	c	511	CLA	C13-C15-C16-C17
31	r	612	CLA	C10-C11-C12-C13
31	s	610	CLA	C5-C6-C7-C8
31	y	612	CLA	C15-C16-C17-C18
31	A1	410	CLA	C5-C6-C7-C8
31	b1	613	CLA	C10-C11-C12-C13
31	b1	614	CLA	C15-C16-C17-C18
31	c1	503	CLA	C13-C15-C16-C17
31	d1	402	CLA	C15-C16-C17-C18
31	n1	603	CLA	C8-C10-C11-C12
31	y1	610	CLA	C8-C10-C11-C12
41	s	624	LHG	C30-C31-C32-C33
55	R1	625	LMT	O5B-C5B-C6B-O6B
31	B	614	CLA	O1A-CGA-O2A-C1
31	G	603	CLA	O1A-CGA-O2A-C1
31	S	604	CLA	O1A-CGA-O2A-C1
31	b	604	CLA	O1A-CGA-O2A-C1
31	B1	602	CLA	O1A-CGA-O2A-C1
31	R1	602	CLA	O1A-CGA-O2A-C1
31	b1	604	CLA	O1A-CGA-O2A-C1
31	b1	613	CLA	O1A-CGA-O2A-C1
52	S1	626	3PH	O32-C31-O31-C3
31	A	406	CLA	CBD-CGD-O2D-CED
34	c	626	SQD	O5-C1-O6-C44
34	a1	412	SQD	O5-C1-O6-C44
34	m1	101	SQD	O5-C1-O6-C44
40	C1	519	DGD	O6E-C1E-O5D-C6D
31	B	604	CLA	C10-C11-C12-C13
31	Y	611	CLA	C10-C11-C12-C13
31	b	608	CLA	C15-C16-C17-C18
31	c	505	CLA	C10-C11-C12-C13
31	c	509	CLA	C15-C16-C17-C18
31	B1	607	CLA	C10-C11-C12-C13
44	d	405	PL9	C39-C41-C42-C43
44	D1	405	PL9	C29-C31-C32-C33
44	D1	405	PL9	C39-C41-C42-C43
44	d1	405	PL9	C34-C36-C37-C38
44	d1	405	PL9	C39-C41-C42-C43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	c1	525	LHG	C33-C34-C35-C36
41	D	410	LHG	C7-C8-C9-C10
41	G1	624	LHG	C23-C24-C25-C26
54	I1	102	4RF	C22-C24-C25-C26
33	B1	619	BCR	C10-C11-C12-C13
33	c1	515	BCR	C10-C11-C12-C13
49	N	622	XAT	C10-C11-C12-C13
49	N	622	XAT	C30-C31-C32-C33
49	R	621	XAT	C30-C31-C32-C33
49	n	622	XAT	C10-C11-C12-C13
49	r1	621	XAT	C30-C31-C32-C33
50	N	623	NEX	C10-C11-C12-C13
50	R	622	NEX	C30-C31-C32-C33
50	r	623	NEX	C30-C31-C32-C33
50	y	623	NEX	C30-C31-C32-C33
50	N1	623	NEX	C10-C11-C12-C13
50	R1	622	NEX	C30-C31-C32-C33
50	S1	623	NEX	C30-C31-C32-C33
50	Y1	623	NEX	C10-C11-C12-C13
50	r1	622	NEX	C30-C31-C32-C33
50	y1	623	NEX	C10-C11-C12-C13
35	D	411	LMG	C35-C36-C37-C38
35	d	411	LMG	C35-C36-C37-C38
41	S	624	LHG	C30-C31-C32-C33
35	b1	622	LMG	O6-C5-C6-O5
41	D	408	LHG	O2-C2-C3-O3
41	G1	624	LHG	O2-C2-C3-O3
34	b1	621	SQD	O49-C7-O47-C45
38	c	524	DGA	OB1-CB1-OG2-CG2
31	B	608	CLA	C3-C5-C6-C7
31	c	511	CLA	C3-C5-C6-C7
47	G1	608	CHL	C2A-CAA-CBA-CGA
31	B	609	CLA	C5-C6-C7-C8
31	B	614	CLA	C13-C15-C16-C17
31	C	504	CLA	C8-C10-C11-C12
31	C	506	CLA	C8-C10-C11-C12
31	C	507	CLA	C13-C15-C16-C17
31	R	608	CLA	C8-C10-C11-C12
31	S	604	CLA	C5-C6-C7-C8
31	Y	604	CLA	C8-C10-C11-C12
31	Y	612	CLA	C10-C11-C12-C13
31	c	506	CLA	C13-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B1	602	CLA	C15-C16-C17-C18
31	B1	608	CLA	C8-C10-C11-C12
31	C1	506	CLA	C5-C6-C7-C8
31	C1	512	CLA	C15-C16-C17-C18
31	D1	403	CLA	C8-C10-C11-C12
31	N1	603	CLA	C5-C6-C7-C8
31	G1	602	CLA	C13-C15-C16-C17
31	Y1	604	CLA	C8-C10-C11-C12
31	Y1	610	CLA	C8-C10-C11-C12
31	Y1	613	CLA	C10-C11-C12-C13
31	b1	605	CLA	C8-C10-C11-C12
31	b1	607	CLA	C8-C10-C11-C12
31	b1	608	CLA	C15-C16-C17-C18
31	c1	505	CLA	C10-C11-C12-C13
31	c1	506	CLA	C5-C6-C7-C8
31	y1	610	CLA	C13-C15-C16-C17
47	n1	609	CHL	C15-C16-C17-C18
31	C	503	CLA	CBA-CGA-O2A-C1
31	S1	603	CLA	CBA-CGA-O2A-C1
31	c1	503	CLA	CBA-CGA-O2A-C1
31	c1	510	CLA	CBA-CGA-O2A-C1
31	r1	612	CLA	CBA-CGA-O2A-C1
41	d	410	LHG	C25-C26-C27-C28
31	b	612	CLA	O1A-CGA-O2A-C1
31	c	507	CLA	O1A-CGA-O2A-C1
31	a1	405	CLA	O1A-CGA-O2A-C1
31	c1	508	CLA	O1A-CGA-O2A-C1
40	C	520	DGD	O1A-C1A-O1G-C1G
32	a	408	PHO	O1D-CGD-O2D-CED
31	B	610	CLA	C15-C16-C17-C18
31	C	506	CLA	C10-C11-C12-C13
31	C	507	CLA	C8-C10-C11-C12
31	C	509	CLA	C13-C15-C16-C17
31	R	608	CLA	C5-C6-C7-C8
31	S	602	CLA	C10-C11-C12-C13
31	b	604	CLA	C15-C16-C17-C18
31	b	614	CLA	C15-C16-C17-C18
31	b	617	CLA	C5-C6-C7-C8
31	c	508	CLA	C8-C10-C11-C12
31	c	508	CLA	C15-C16-C17-C18
31	g	610	CLA	C15-C16-C17-C18
31	y	612	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C1	507	CLA	C13-C15-C16-C17
31	C1	508	CLA	C10-C11-C12-C13
31	N1	603	CLA	C8-C10-C11-C12
31	R1	612	CLA	C10-C11-C12-C13
31	Y1	603	CLA	C8-C10-C11-C12
31	Y1	611	CLA	C15-C16-C17-C18
31	b1	602	CLA	C13-C15-C16-C17
31	b1	607	CLA	C13-C15-C16-C17
31	c1	504	CLA	C10-C11-C12-C13
31	c1	505	CLA	C5-C6-C7-C8
31	n1	602	CLA	C5-C6-C7-C8
31	n1	603	CLA	C13-C15-C16-C17
31	g1	611	CLA	C5-C6-C7-C8
31	s1	613	CLA	C5-C6-C7-C8
31	y1	603	CLA	C15-C16-C17-C18
47	g1	607	CHL	C5-C6-C7-C8
31	C1	503	CLA	O1A-CGA-O2A-C1
31	c1	504	CLA	O1A-CGA-O2A-C1
38	b	623	DGA	OA1-CA1-OG1-CG1
51	S1	625	LPX	O5-C4-C5-O6
34	M1	101	SQD	C8-C7-O47-C45
34	b1	621	SQD	C8-C7-O47-C45
35	C1	521	LMG	C11-C10-O7-C8
35	C1	523	LMG	C11-C10-O7-C8
41	S1	624	LHG	C8-C7-O7-C5
54	i1	101	4RF	C33-C34-C35-C36
31	B	602	CLA	C5-C6-C7-C8
31	C	503	CLA	C5-C6-C7-C8
31	C	505	CLA	C13-C15-C16-C17
31	C	509	CLA	C10-C11-C12-C13
31	N	603	CLA	C5-C6-C7-C8
31	G	613	CLA	C13-C15-C16-C17
31	Y	602	CLA	C13-C15-C16-C17
31	b	608	CLA	C8-C10-C11-C12
31	b	616	CLA	C5-C6-C7-C8
31	c	506	CLA	C10-C11-C12-C13
31	d	403	CLA	C15-C16-C17-C18
31	B1	613	CLA	C10-C11-C12-C13
31	C1	505	CLA	C8-C10-C11-C12
31	C1	508	CLA	C13-C15-C16-C17
31	C1	510	CLA	C15-C16-C17-C18
31	R1	602	CLA	C10-C11-C12-C13

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R1	608	CLA	C10-C11-C12-C13
31	R1	609	CLA	C10-C11-C12-C13
31	Y1	612	CLA	C5-C6-C7-C8
31	r1	612	CLA	C10-C11-C12-C13
41	C	525	LHG	C3-O3-P-O6
41	C	525	LHG	C4-O6-P-O3
41	D	408	LHG	C4-O6-P-O3
41	D	409	LHG	C3-O3-P-O6
41	G	630	LHG	C4-O6-P-O3
41	S	624	LHG	C4-O6-P-O3
41	d	410	LHG	C3-O3-P-O6
41	d	410	LHG	C4-O6-P-O3
41	l	101	LHG	C3-O3-P-O6
41	g	624	LHG	C4-O6-P-O3
41	s	624	LHG	C4-O6-P-O3
41	y	624	LHG	C3-O3-P-O6
41	y	624	LHG	C4-O6-P-O3
41	C1	525	LHG	C4-O6-P-O3
41	D1	408	LHG	C3-O3-P-O6
41	D1	408	LHG	C4-O6-P-O3
41	N1	624	LHG	C4-O6-P-O3
41	G1	624	LHG	C4-O6-P-O3
41	S1	624	LHG	C4-O6-P-O3
41	Y1	624	LHG	C4-O6-P-O3
41	c1	525	LHG	C4-O6-P-O3
41	d1	410	LHG	C3-O3-P-O6
41	d1	410	LHG	C4-O6-P-O3
41	n1	624	LHG	C4-O6-P-O3
41	g1	624	LHG	C4-O6-P-O3
51	s	625	LPX	C3-O1-P1-O2
51	s	625	LPX	C1-O2-P1-O1
57	y1	627	PTY	C3-O11-P1-O14
34	b1	626	SQD	C23-C24-C25-C26
54	k1	101	4RF	C41-C43-C44-C45
31	c1	508	CLA	C3-C5-C6-C7
35	d1	411	LMG	C4-C5-C6-O5
54	I1	102	4RF	C33-C34-C35-C36
31	C1	510	CLA	CBA-CGA-O2A-C1
31	R1	610	CLA	CBA-CGA-O2A-C1
31	g1	603	CLA	CBA-CGA-O2A-C1
31	g1	610	CLA	CBA-CGA-O2A-C1
31	B	616	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	507	CLA	C8-C10-C11-C12
31	B1	612	CLA	C15-C16-C17-C18
31	b1	615	CLA	C10-C11-C12-C13
38	C1	524	DGA	CCB-CDB-CEB-CFB
38	C1	524	DGA	CB1-CB2-CB3-CB4
31	d	402	CLA	O1D-CGD-O2D-CED
31	s	614	CLA	O1D-CGD-O2D-CED
41	c	625	LHG	C1-C2-C3-O3
41	y	624	LHG	C1-C2-C3-O3
41	S1	624	LHG	C1-C2-C3-O3
34	M1	101	SQD	O49-C7-O47-C45
35	C1	521	LMG	O9-C10-O7-C8
35	C1	523	LMG	O9-C10-O7-C8
40	c	519	DGD	O1B-C1B-O2G-C2G
41	g	624	LHG	O9-C7-O7-C5
57	Y1	626	PTY	O10-C8-O7-C6
31	c	513	CLA	C4-C3-C5-C6
31	n	603	CLA	C4-C3-C5-C6
47	n1	601	CHL	C4-C3-C5-C6
31	b	604	CLA	C2-C3-C5-C6
31	A	406	CLA	C5-C6-C7-C8
31	B	602	CLA	C13-C15-C16-C17
31	B	606	CLA	C15-C16-C17-C18
31	B	614	CLA	C10-C11-C12-C13
31	c	507	CLA	C13-C15-C16-C17
31	y	610	CLA	C10-C11-C12-C13
31	B1	608	CLA	C15-C16-C17-C18
31	C1	508	CLA	C15-C16-C17-C18
31	b1	617	CLA	C5-C6-C7-C8
31	d1	402	CLA	C13-C15-C16-C17
41	c1	525	LHG	O10-C23-O8-C6
31	C	505	CLA	C2A-CAA-CBA-CGA
31	N	602	CLA	C2A-CAA-CBA-CGA
31	Y	613	CLA	C2A-CAA-CBA-CGA
31	c	505	CLA	C2A-CAA-CBA-CGA
31	g	610	CLA	C2A-CAA-CBA-CGA
31	r	612	CLA	C2A-CAA-CBA-CGA
31	s	604	CLA	C2A-CAA-CBA-CGA
31	C1	507	CLA	C2A-CAA-CBA-CGA
31	R1	610	CLA	C2A-CAA-CBA-CGA
31	S1	613	CLA	C2A-CAA-CBA-CGA
31	n1	602	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	r1	604	CLA	C2A-CAA-CBA-CGA
31	r1	610	CLA	C2A-CAA-CBA-CGA
47	Y	607	CHL	C2A-CAA-CBA-CGA
47	n	605	CHL	C2A-CAA-CBA-CGA
47	g	605	CHL	C2A-CAA-CBA-CGA
47	y1	607	CHL	C2A-CAA-CBA-CGA
31	B	604	CLA	C16-C17-C18-C20
31	S	613	CLA	C6-C7-C8-C10
31	s	613	CLA	C6-C7-C8-C10
31	C1	507	CLA	C16-C17-C18-C20
31	y1	614	CLA	C16-C17-C18-C19
31	Y1	614	CLA	C3-C5-C6-C7
31	B	613	CLA	CBA-CGA-O2A-C1
31	C	507	CLA	CBA-CGA-O2A-C1
31	R	602	CLA	CBA-CGA-O2A-C1
31	R	604	CLA	CBA-CGA-O2A-C1
31	Y	602	CLA	CBA-CGA-O2A-C1
31	g	610	CLA	CBA-CGA-O2A-C1
31	Y1	610	CLA	CBA-CGA-O2A-C1
31	b1	611	CLA	CBA-CGA-O2A-C1
31	b1	612	CLA	CBA-CGA-O2A-C1
31	y1	614	CLA	CBA-CGA-O2A-C1
41	d1	410	LHG	C24-C23-O8-C6
51	S	625	LPX	C7-C6-O6-C5
31	B	607	CLA	C13-C15-C16-C17
31	b	614	CLA	C8-C10-C11-C12
31	N1	603	CLA	C15-C16-C17-C18
31	a1	405	CLA	C10-C11-C12-C13
31	r1	610	CLA	C8-C10-C11-C12
42	C	527	LMK	O7-C10-C11-C12
42	c	627	LMK	O8-C28-C29-C30
31	Y	611	CLA	C8-C10-C11-C12
31	r1	603	CLA	C8-C10-C11-C12
47	G1	607	CHL	C5-C6-C7-C8
33	A1	411	BCR	C9-C10-C11-C12
33	C1	517	BCR	C9-C10-C11-C12
37	B	620	C7Z	C9-C10-C11-C12
37	b	620	C7Z	C29-C30-C31-C32
50	S	622	NEX	C13-C14-C15-C35
34	C	526	SQD	C7-C8-C9-C10
41	d	410	LHG	C7-C8-C9-C10
34	C	526	SQD	C32-C33-C34-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	H1	102	LMG	C30-C31-C32-C33
35	W1	201	LMG	C32-C33-C34-C35
38	J1	101	DGA	CA6-CA7-CA8-CA9
38	J1	101	DGA	CB7-CB8-CB9-CAB
41	d	408	LHG	C25-C26-C27-C28
41	n	624	LHG	C13-C14-C15-C16
41	L1	101	LHG	C28-C29-C30-C31
42	C1	527	LMK	C12-C13-C14-C15
53	Y1	625	SPH	C14-C15-C16-C17
35	A1	413	LMG	C11-C10-O7-C8
41	D	408	LHG	C8-C7-O7-C5
41	D1	409	LHG	C8-C7-O7-C5
41	N1	624	LHG	C8-C7-O7-C5
41	G1	624	LHG	C8-C7-O7-C5
31	S	609	CLA	C10-C11-C12-C13
31	Y	612	CLA	C8-C10-C11-C12
31	c1	506	CLA	C15-C16-C17-C18
31	r1	610	CLA	C10-C11-C12-C13
31	y1	602	CLA	C13-C15-C16-C17
33	c	514	BCR	C11-C10-C9-C34
49	R	621	XAT	C40-C33-C34-C35
49	r	622	XAT	C20-C13-C14-C15
49	r	622	XAT	C40-C33-C34-C35
49	R1	621	XAT	C20-C13-C14-C15
50	G	623	NEX	C39-C29-C30-C31
50	R	622	NEX	C39-C29-C30-C31
50	R	622	NEX	C40-C33-C34-C35
50	S	622	NEX	C40-C33-C34-C35
50	r	623	NEX	C20-C13-C14-C15
50	r	623	NEX	C39-C29-C30-C31
50	N1	623	NEX	C39-C29-C30-C31
50	R1	622	NEX	C39-C29-C30-C31
50	Y1	623	NEX	C11-C10-C9-C19
50	Y1	623	NEX	C20-C13-C14-C15
50	g1	623	NEX	C39-C29-C30-C31
50	r1	622	NEX	C39-C29-C30-C31
50	r1	622	NEX	C40-C33-C34-C35
50	s1	623	NEX	C39-C29-C30-C31
50	y1	623	NEX	C39-C29-C30-C31
31	n	604	CLA	C3-C5-C6-C7
31	c1	512	CLA	C3-C5-C6-C7
34	C1	526	SQD	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	B	622	LMG	C15-C16-C17-C18
35	C	521	LMG	C29-C30-C31-C32
38	b	623	DGA	CA6-CA7-CA8-CA9
38	b	623	DGA	CDB-CEB-CFB-CGB
38	C1	524	DGA	CA9-CAA-CBA-CCA
40	c1	520	DGD	CCB-CDB-CEB-CFB
41	c	625	LHG	C34-C35-C36-C37
41	l	101	LHG	C11-C12-C13-C14
41	y	624	LHG	C11-C10-C9-C8
41	C1	525	LHG	C29-C30-C31-C32
41	D1	408	LHG	C30-C31-C32-C33
41	Y1	624	LHG	C29-C30-C31-C32
41	d1	409	LHG	C25-C26-C27-C28
52	S	626	3PH	C22-C23-C24-C25
52	S	626	3PH	C25-C26-C27-C28
52	S	626	3PH	C3E-C3F-C3G-C3H
52	T1	101	3PH	C28-C29-C2A-C2B
52	t1	101	3PH	C35-C36-C37-C38
55	R1	625	LMT	C4-C5-C6-C7
31	C	513	CLA	C16-C17-C18-C20
31	G	602	CLA	C16-C17-C18-C19
31	R	603	CLA	C11-C12-C13-C15
31	S	602	CLA	C11-C12-C13-C15
31	S	604	CLA	C6-C7-C8-C9
31	Y	602	CLA	C16-C17-C18-C20
31	c	504	CLA	C16-C17-C18-C20
31	c	507	CLA	C16-C17-C18-C20
31	r	609	CLA	C11-C12-C13-C15
31	y	610	CLA	C16-C17-C18-C20
31	B1	609	CLA	C16-C17-C18-C19
31	C1	501	CLA	C16-C17-C18-C19
31	b1	602	CLA	C16-C17-C18-C20
31	c1	501	CLA	C16-C17-C18-C20
31	c1	507	CLA	C16-C17-C18-C19
31	n1	602	CLA	C16-C17-C18-C19
31	G1	603	CLA	CBA-CGA-O2A-C1
31	Y1	614	CLA	CBA-CGA-O2A-C1
41	d	410	LHG	C24-C23-O8-C6
51	s1	625	LPX	C7-C6-O6-C5
51	S1	625	LPX	C3-C4-C5-O6
35	b1	622	LMG	C12-C13-C14-C15
38	c	524	DGA	CB4-CB5-CB6-CB7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	C1	524	DGA	CA2-CA3-CA4-CA5
38	j1	101	DGA	CA2-CA3-CA4-CA5
40	C	519	DGD	C2B-C3B-C4B-C5B
40	C1	520	DGD	C4B-C5B-C6B-C7B
41	D	408	LHG	C13-C14-C15-C16
41	Y	624	LHG	C11-C12-C13-C14
41	d	408	LHG	C28-C29-C30-C31
41	d	408	LHG	C33-C34-C35-C36
41	l	101	LHG	C25-C26-C27-C28
41	y	624	LHG	C30-C31-C32-C33
52	S1	626	3PH	C24-C25-C26-C27
53	y1	625	SPH	C11-C10-C9-C8
55	r1	625	LMT	C11-C10-C9-C8
53	y	625	SPH	O3-C3-C4-C5
31	C	508	CLA	O1D-CGD-O2D-CED
35	A1	413	LMG	O9-C10-O7-C8
41	D	408	LHG	O9-C7-O7-C5
41	C1	525	LHG	O9-C7-O7-C5
41	D1	409	LHG	O9-C7-O7-C5
41	N1	624	LHG	O9-C7-O7-C5
41	G1	624	LHG	O9-C7-O7-C5
41	S1	624	LHG	O9-C7-O7-C5
31	s	610	CLA	C10-C11-C12-C13
31	G1	602	CLA	C15-C16-C17-C18
31	Y1	612	CLA	C10-C11-C12-C13
41	D1	409	LHG	C7-C8-C9-C10
34	b	621	SQD	C30-C31-C32-C33
35	H1	102	LMG	C13-C14-C15-C16
38	B	625	DGA	CB7-CB8-CB9-CAB
38	c	524	DGA	CB5-CB6-CB7-CB8
38	J1	101	DGA	CB3-CB4-CB5-CB6
40	C	523	DGD	C7B-C8B-C9B-CAB
40	c	519	DGD	C9B-CAB-CBB-CCB
41	D	409	LHG	C13-C14-C15-C16
41	D1	408	LHG	C28-C29-C30-C31
41	D1	408	LHG	C33-C34-C35-C36
41	S1	624	LHG	C28-C29-C30-C31
52	s	626	3PH	C3B-C3C-C3D-C3E
52	S1	626	3PH	C2B-C2C-C2D-C2E
52	t1	101	3PH	C27-C28-C29-C2A
52	s1	626	3PH	C2A-C2B-C2C-C2D
41	C1	525	LHG	C2-C3-O3-P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C	507	CLA	O1A-CGA-O2A-C1
31	R1	610	CLA	O1A-CGA-O2A-C1
40	C	518	DGD	O1A-C1A-O1G-C1G
34	B1	626	SQD	C13-C14-C15-C16
35	c	521	LMG	C11-C12-C13-C14
38	C	524	DGA	CB4-CB5-CB6-CB7
38	B1	625	DGA	CA7-CA8-CA9-CAA
41	N	624	LHG	C15-C16-C17-C18
41	D1	408	LHG	C29-C30-C31-C32
41	N1	624	LHG	C28-C29-C30-C31
41	c1	525	LHG	C28-C29-C30-C31
41	s1	624	LHG	C9-C10-C11-C12
52	S	626	3PH	C35-C36-C37-C38
52	T1	101	3PH	C38-C39-C3A-C3B
54	K1	101	4RF	C44-C45-C46-C47
57	Y1	626	PTY	C40-C41-C42-C43
31	B1	615	CLA	C10-C11-C12-C13
34	b	621	SQD	C26-C27-C28-C29
38	C1	524	DGA	CEA-CFA-CGA-CHA
38	c1	524	DGA	CA4-CA5-CA6-CA7
41	d	410	LHG	C26-C27-C28-C29
41	S1	624	LHG	C11-C12-C13-C14
41	c1	525	LHG	C13-C14-C15-C16
41	c1	525	LHG	C29-C30-C31-C32
42	C1	527	LMK	C31-C32-C33-C34
54	k1	101	4RF	C32-C33-C34-C35
54	k1	101	4RF	C43-C44-C45-C46
40	B1	623	DGD	C4D-C5D-C6D-O5D
41	D	409	LHG	C7-C8-C9-C10
41	Y1	624	LHG	C23-C24-C25-C26
31	Y	604	CLA	O1D-CGD-O2D-CED
31	C1	508	CLA	O1D-CGD-O2D-CED
33	C	515	BCR	C11-C10-C9-C8
33	c	514	BCR	C11-C10-C9-C8
34	B1	621	SQD	C2-C1-O6-C44
34	m1	101	SQD	C2-C1-O6-C44
35	A1	413	LMG	C2-C1-O1-C7
35	b1	622	LMG	C2-C1-O1-C7
35	c1	523	LMG	C2-C1-O1-C7
40	C1	519	DGD	C2E-C1E-O5D-C6D
40	c1	519	DGD	C2E-C1E-O5D-C6D
49	R	621	XAT	C32-C33-C34-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
49	r	622	XAT	C12-C13-C14-C15
49	r	622	XAT	C32-C33-C34-C35
49	R1	621	XAT	C12-C13-C14-C15
50	G	623	NEX	C28-C29-C30-C31
50	R	622	NEX	C28-C29-C30-C31
50	R	622	NEX	C32-C33-C34-C35
50	S	622	NEX	C32-C33-C34-C35
50	r	623	NEX	C12-C13-C14-C15
50	r	623	NEX	C28-C29-C30-C31
50	N1	623	NEX	C28-C29-C30-C31
50	R1	622	NEX	C28-C29-C30-C31
50	Y1	623	NEX	C11-C10-C9-C8
50	Y1	623	NEX	C12-C13-C14-C15
50	g1	623	NEX	C28-C29-C30-C31
50	r1	622	NEX	C28-C29-C30-C31
50	r1	622	NEX	C32-C33-C34-C35
50	s1	623	NEX	C28-C29-C30-C31
50	y1	623	NEX	C28-C29-C30-C31
31	B1	606	CLA	CBA-CGA-O2A-C1
41	C	525	LHG	C24-C23-O8-C6
41	C1	525	LHG	C24-C23-O8-C6
41	D1	410	LHG	C24-C23-O8-C6
54	i1	101	4RF	C43-C41-O40-C39
34	b1	621	SQD	C10-C11-C12-C13
35	C1	523	LMG	C18-C19-C20-C21
38	B	625	DGA	CDA-CEA-CFA-CGA
38	C	524	DGA	CCB-CDB-CEB-CFB
38	C1	524	DGA	CBB-CAB-CB9-CB8
41	N	624	LHG	C13-C14-C15-C16
41	G	630	LHG	C28-C29-C30-C31
41	G	630	LHG	C31-C32-C33-C34
52	S1	626	3PH	C22-C23-C24-C25
52	t1	101	3PH	C22-C23-C24-C25
54	K1	101	4RF	C45-C46-C47-C48
31	G	613	CLA	C8-C10-C11-C12
31	B1	611	CLA	C15-C16-C17-C18
31	n1	613	CLA	C13-C15-C16-C17
31	g	610	CLA	O1A-CGA-O2A-C1
31	b1	611	CLA	O1A-CGA-O2A-C1
31	B	617	CLA	C16-C17-C18-C19
31	S	609	CLA	C11-C12-C13-C14
31	c	513	CLA	C16-C17-C18-C19

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	n	604	CLA	C16-C17-C18-C20
31	g	602	CLA	C16-C17-C18-C20
31	s	613	CLA	C6-C7-C8-C9
31	R1	608	CLA	C11-C12-C13-C14
31	S1	602	CLA	C11-C12-C13-C14
31	Y1	614	CLA	C16-C17-C18-C19
47	Y	607	CHL	C4-C3-C5-C6
34	a	412	SQD	C14-C15-C16-C17
34	A1	412	SQD	C13-C14-C15-C16
38	C	524	DGA	CA4-CA5-CA6-CA7
38	c1	524	DGA	CB7-CB8-CB9-CAB
40	c	519	DGD	C3B-C4B-C5B-C6B
41	L	101	LHG	C9-C10-C11-C12
41	d	409	LHG	C29-C30-C31-C32
41	l	101	LHG	C13-C14-C15-C16
41	g	624	LHG	C31-C32-C33-C34
41	L1	101	LHG	C25-C26-C27-C28
41	N1	624	LHG	C33-C34-C35-C36
41	d1	408	LHG	C11-C12-C13-C14
41	s1	624	LHG	C11-C12-C13-C14
41	y1	624	LHG	C16-C17-C18-C19
41	y1	624	LHG	C29-C30-C31-C32
53	Y1	625	SPH	C11-C10-C9-C8
54	k1	101	4RF	C34-C35-C36-C37
44	D1	405	PL9	C18-C19-C21-C22
47	n1	601	CHL	C2-C3-C5-C6
31	B	606	CLA	C11-C12-C13-C14
31	C	503	CLA	C11-C12-C13-C14
31	C	503	CLA	C14-C13-C15-C16
31	C	512	CLA	C11-C12-C13-C14
31	N	604	CLA	C14-C13-C15-C16
31	N	613	CLA	C14-C13-C15-C16
31	Y	602	CLA	C11-C12-C13-C14
31	b	606	CLA	C11-C12-C13-C14
31	c	505	CLA	C11-C10-C8-C9
31	c	509	CLA	C11-C10-C8-C9
31	n	602	CLA	C11-C10-C8-C9
31	s	611	CLA	C6-C7-C8-C9
31	y	602	CLA	C11-C12-C13-C14
31	y	613	CLA	C11-C12-C13-C14
31	B1	611	CLA	C11-C10-C8-C9
31	B1	613	CLA	C14-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B1	615	CLA	C6-C7-C8-C9
31	C1	512	CLA	C14-C13-C15-C16
31	N1	604	CLA	C6-C7-C8-C9
31	b1	613	CLA	C14-C13-C15-C16
31	n1	610	CLA	C6-C7-C8-C9
31	r1	602	CLA	C6-C7-C8-C9
47	N	607	CHL	C11-C12-C13-C14
47	y1	606	CHL	C6-C7-C8-C9
41	N	624	LHG	C7-C8-C9-C10
41	D1	410	LHG	C7-C8-C9-C10
41	d1	408	LHG	C7-C8-C9-C10
34	M1	101	SQD	C24-C25-C26-C27
35	C1	523	LMG	C32-C33-C34-C35
38	B	625	DGA	CB5-CB6-CB7-CB8
38	b	623	DGA	CA4-CA5-CA6-CA7
38	B1	625	DGA	CB5-CB6-CB7-CB8
38	C1	524	DGA	CA4-CA5-CA6-CA7
38	C1	524	DGA	CB7-CB8-CB9-CAB
38	b1	625	DGA	CA6-CA7-CA8-CA9
38	b1	625	DGA	CB7-CB8-CB9-CAB
40	C	520	DGD	C3B-C4B-C5B-C6B
41	Y	624	LHG	C30-C31-C32-C33
41	Y	624	LHG	C32-C33-C34-C35
41	D1	408	LHG	C26-C27-C28-C29
41	d1	408	LHG	C13-C14-C15-C16
41	d1	409	LHG	C11-C12-C13-C14
41	d1	409	LHG	C13-C14-C15-C16
41	n1	624	LHG	C33-C34-C35-C36
41	y1	624	LHG	C31-C32-C33-C34
51	S1	625	LPX	C7-C8-C9-C10
52	b1	624	3PH	C2E-C2F-C2G-C2H
53	A1	414	SPH	C11-C12-C13-C14
54	i1	101	4RF	C07-C08-C09-C10
31	c	509	CLA	C8-C10-C11-C12
31	c	512	CLA	C8-C10-C11-C12
31	b1	610	CLA	C13-C15-C16-C17
31	y1	612	CLA	C5-C6-C7-C8
47	s	608	CHL	C5-C6-C7-C8
31	R	604	CLA	C2A-CAA-CBA-CGA
31	S	604	CLA	C2A-CAA-CBA-CGA
31	a	407	CLA	C2A-CAA-CBA-CGA
31	c	512	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B1	602	CLA	C2A-CAA-CBA-CGA
31	B1	613	CLA	C2A-CAA-CBA-CGA
31	b1	607	CLA	C2A-CAA-CBA-CGA
31	b1	613	CLA	C2A-CAA-CBA-CGA
31	b1	617	CLA	C2A-CAA-CBA-CGA
47	N1	606	CHL	C2A-CAA-CBA-CGA
31	C	503	CLA	O1A-CGA-O2A-C1
31	R	602	CLA	O1A-CGA-O2A-C1
31	S1	603	CLA	O1A-CGA-O2A-C1
31	c1	503	CLA	O1A-CGA-O2A-C1
31	r1	612	CLA	O1A-CGA-O2A-C1
33	C1	514	BCR	C11-C12-C13-C35
33	C1	516	BCR	C37-C22-C23-C24
33	c1	515	BCR	C7-C8-C9-C34
46	h1	101	RRX	C11-C12-C13-C35
35	D1	411	LMG	C29-C30-C31-C32
38	B1	625	DGA	CB3-CB4-CB5-CB6
41	Y1	624	LHG	C31-C32-C33-C34
41	c1	525	LHG	C14-C15-C16-C17
41	C	525	LHG	O1-C1-C2-C3
41	D	409	LHG	O1-C1-C2-C3
41	L	101	LHG	O1-C1-C2-C3
41	N	624	LHG	O1-C1-C2-C3
41	S	624	LHG	O1-C1-C2-C3
41	Y	624	LHG	O1-C1-C2-C3
41	d	409	LHG	O1-C1-C2-C3
41	d	410	LHG	O1-C1-C2-C3
41	l	101	LHG	O1-C1-C2-C3
41	n	624	LHG	O1-C1-C2-C3
41	C1	525	LHG	O1-C1-C2-C3
41	D1	409	LHG	O1-C1-C2-C3
41	G1	624	LHG	O1-C1-C2-C3
41	Y1	624	LHG	O1-C1-C2-C3
41	c1	525	LHG	O1-C1-C2-C3
41	g1	624	LHG	O1-C1-C2-C3
33	c1	515	BCR	C7-C8-C9-C10
46	h	101	RRX	C17-C18-C19-C20
46	h1	101	RRX	C11-C12-C13-C14
48	y	621	LUT	C31-C32-C33-C34
48	n1	620	LUT	C27-C28-C29-C30
49	R	621	XAT	C7-C8-C9-C10
49	Y1	622	XAT	C27-C28-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
51	s1	625	LPX	O5-C4-C5-O6
31	g	603	CLA	C15-C16-C17-C18
31	n1	613	CLA	C10-C11-C12-C13
31	g1	602	CLA	C5-C6-C7-C8
31	g1	603	CLA	C8-C10-C11-C12
31	s1	603	CLA	C15-C16-C17-C18
41	Y	624	LHG	C8-C7-O7-C5
41	d	410	LHG	C8-C7-O7-C5
34	A1	412	SQD	C12-C13-C14-C15
35	J	101	LMG	C29-C30-C31-C32
40	c	520	DGD	CAB-CBB-CCB-CDB
41	D	410	LHG	C29-C30-C31-C32
41	G	630	LHG	C25-C26-C27-C28
41	c	625	LHG	C13-C14-C15-C16
41	g1	624	LHG	C13-C14-C15-C16
41	y1	624	LHG	C13-C14-C15-C16
55	R1	625	LMT	C11-C10-C9-C8
55	r1	625	LMT	C3-C4-C5-C6
35	B	622	LMG	C28-C29-C30-C31
38	B1	625	DGA	CB1-CB2-CB3-CB4
41	D	409	LHG	C23-C24-C25-C26
41	G	630	LHG	C7-C8-C9-C10
34	A	412	SQD	C24-C25-C26-C27
34	B	621	SQD	C10-C11-C12-C13
34	B	621	SQD	C29-C30-C31-C32
34	c	626	SQD	C28-C29-C30-C31
34	A1	412	SQD	C33-C34-C35-C36
34	B1	621	SQD	C25-C26-C27-C28
34	b1	626	SQD	C34-C35-C36-C37
34	c1	526	SQD	C17-C18-C19-C20
35	a	413	LMG	C33-C34-C35-C36
35	c	521	LMG	C16-C17-C18-C19
38	C	524	DGA	CB5-CB6-CB7-CB8
38	c1	524	DGA	CA6-CA7-CA8-CA9
40	c	523	DGD	C2A-C3A-C4A-C5A
41	D	408	LHG	C29-C30-C31-C32
41	Y	624	LHG	C28-C29-C30-C31
41	d	408	LHG	C13-C14-C15-C16
41	d	409	LHG	C11-C12-C13-C14
41	y	624	LHG	C13-C14-C15-C16
41	D1	409	LHG	C11-C12-C13-C14
41	N1	624	LHG	C27-C28-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	N1	624	LHG	C31-C32-C33-C34
41	G1	624	LHG	C11-C10-C9-C8
41	s1	624	LHG	C13-C14-C15-C16
41	y1	624	LHG	C28-C29-C30-C31
52	s	626	3PH	C23-C24-C25-C26
52	T1	101	3PH	C27-C28-C29-C2A
52	t1	101	3PH	C3B-C3C-C3D-C3E
52	s1	626	3PH	C23-C24-C25-C26
53	Y	625	SPH	C6-C7-C8-C9
53	y	625	SPH	C7-C8-C9-C10
54	I1	102	4RF	C07-C08-C09-C10
54	K1	101	4RF	C26-C27-C28-C29
57	y1	626	PTY	C37-C38-C39-C40
31	b1	612	CLA	O1A-CGA-O2A-C1
31	B	604	CLA	C16-C17-C18-C19
31	C	504	CLA	C16-C17-C18-C19
31	C	504	CLA	C16-C17-C18-C20
31	C	507	CLA	C16-C17-C18-C20
31	C	513	CLA	C16-C17-C18-C19
31	G	613	CLA	C16-C17-C18-C19
31	R	603	CLA	C11-C12-C13-C14
31	R	608	CLA	C11-C12-C13-C15
31	R	609	CLA	C11-C12-C13-C14
31	R	609	CLA	C11-C12-C13-C15
31	S	602	CLA	C11-C12-C13-C14
31	S	604	CLA	C6-C7-C8-C10
31	Y	602	CLA	C16-C17-C18-C19
31	n	602	CLA	C16-C17-C18-C19
31	n	602	CLA	C16-C17-C18-C20
31	r	609	CLA	C11-C12-C13-C14
31	y	604	CLA	C16-C17-C18-C19
31	y	604	CLA	C16-C17-C18-C20
31	y	610	CLA	C16-C17-C18-C19
31	y	611	CLA	C16-C17-C18-C19
31	B1	602	CLA	C16-C17-C18-C19
31	C1	507	CLA	C16-C17-C18-C19
31	C1	513	CLA	C16-C17-C18-C19
31	C1	513	CLA	C16-C17-C18-C20
31	D1	402	CLA	C16-C17-C18-C19
31	D1	402	CLA	C16-C17-C18-C20
31	Y1	613	CLA	C16-C17-C18-C20
31	b1	602	CLA	C16-C17-C18-C19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c1	509	CLA	C16-C17-C18-C19
31	c1	509	CLA	C16-C17-C18-C20
31	n1	602	CLA	C16-C17-C18-C20
31	g1	602	CLA	C16-C17-C18-C20
31	r1	608	CLA	C11-C12-C13-C15
47	s1	608	CHL	C11-C12-C13-C14
35	c1	523	LMG	O6-C1-O1-C7
40	c1	519	DGD	O6E-C1E-O5D-C6D
31	C	506	CLA	C13-C15-C16-C17
31	N	613	CLA	C10-C11-C12-C13
31	b	607	CLA	C8-C10-C11-C12
31	C1	501	CLA	C15-C16-C17-C18
31	C1	511	CLA	C5-C6-C7-C8
31	c1	509	CLA	C10-C11-C12-C13
31	c1	510	CLA	C8-C10-C11-C12
31	s1	603	CLA	C5-C6-C7-C8
47	y	606	CHL	C15-C16-C17-C18
34	b	621	SQD	C14-C15-C16-C17
34	A1	412	SQD	C31-C32-C33-C34
34	B1	626	SQD	C11-C12-C13-C14
35	A	413	LMG	C30-C31-C32-C33
38	b	623	DGA	CCA-CDA-CEA-CFA
38	b1	625	DGA	CCB-CDB-CEB-CFB
38	j1	101	DGA	CB5-CB6-CB7-CB8
40	C1	518	DGD	C3A-C4A-C5A-C6A
41	D	409	LHG	C11-C12-C13-C14
41	D	409	LHG	C18-C19-C20-C21
41	d	408	LHG	C29-C30-C31-C32
41	L1	101	LHG	C13-C14-C15-C16
41	N1	624	LHG	C13-C14-C15-C16
41	c1	525	LHG	C11-C12-C13-C14
41	c1	525	LHG	C26-C27-C28-C29
41	d1	409	LHG	C28-C29-C30-C31
52	S1	626	3PH	C25-C26-C27-C28
52	t1	101	3PH	C38-C39-C3A-C3B
54	K1	101	4RF	C10-C11-C12-C13
56	R1	626	ERG	C13-C17-C20-C22
56	R1	626	ERG	C16-C17-C20-C22
56	r1	626	ERG	C13-C17-C20-C22
31	B1	602	CLA	O1D-CGD-O2D-CED
34	M1	101	SQD	C13-C14-C15-C16
38	B	625	DGA	CA9-CAA-CBA-CCA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	C1	524	DGA	CA7-CA8-CA9-CAA
38	b1	625	DGA	CDB-CEB-CFB-CGB
38	j1	101	DGA	CA5-CA6-CA7-CA8
41	D	408	LHG	C33-C34-C35-C36
41	Y	624	LHG	C13-C14-C15-C16
41	d1	409	LHG	C34-C35-C36-C37
41	g1	624	LHG	C31-C32-C33-C34
52	s	626	3PH	C24-C25-C26-C27
52	s	626	3PH	C25-C26-C27-C28
52	B1	624	3PH	C3C-C3D-C3E-C3F
52	T1	101	3PH	C22-C23-C24-C25
54	k1	101	4RF	C30-C31-C32-C33
35	C	521	LMG	C28-C29-C30-C31
40	c	519	DGD	C1B-C2B-C3B-C4B
41	d	408	LHG	C23-C24-C25-C26
41	g	624	LHG	C7-C8-C9-C10
52	B1	624	3PH	C31-C32-C33-C34
31	g	602	CLA	C15-C16-C17-C18
31	r	603	CLA	C8-C10-C11-C12
31	S1	611	CLA	C10-C11-C12-C13
31	c1	513	CLA	C10-C11-C12-C13
31	B	613	CLA	O1A-CGA-O2A-C1
31	Y1	610	CLA	O1A-CGA-O2A-C1
31	y1	614	CLA	O1A-CGA-O2A-C1
38	b	623	DGA	CEA-CFA-CGA-CHA
38	b1	625	DGA	CA9-CAA-CBA-CCA
41	L	101	LHG	C13-C14-C15-C16
41	s	624	LHG	C13-C14-C15-C16
41	D1	408	LHG	C13-C14-C15-C16
41	g1	624	LHG	C28-C29-C30-C31
41	s1	624	LHG	C30-C31-C32-C33
31	B	603	CLA	C3-C5-C6-C7
31	R1	612	CLA	C3-C5-C6-C7
54	K1	101	4RF	C15-C16-O18-C19
34	B	621	SQD	C11-C12-C13-C14
35	h	102	LMG	C37-C38-C39-C40
38	b	623	DGA	CB3-CB4-CB5-CB6
41	D	408	LHG	C28-C29-C30-C31
41	n	624	LHG	C26-C27-C28-C29
41	C1	525	LHG	C30-C31-C32-C33
52	S	626	3PH	C24-C25-C26-C27
52	S1	626	3PH	C33-C34-C35-C36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
54	K1	101	4RF	C27-C28-C29-C30
31	B	609	CLA	C3A-C2A-CAA-CBA
31	B	615	CLA	C3A-C2A-CAA-CBA
31	C	513	CLA	C3A-C2A-CAA-CBA
31	D	402	CLA	C3A-C2A-CAA-CBA
31	N	612	CLA	C3A-C2A-CAA-CBA
31	G	603	CLA	C3A-C2A-CAA-CBA
31	G	611	CLA	C3A-C2A-CAA-CBA
31	Y	603	CLA	C3A-C2A-CAA-CBA
31	a	405	CLA	C3A-C2A-CAA-CBA
31	b	609	CLA	C3A-C2A-CAA-CBA
31	b	615	CLA	C3A-C2A-CAA-CBA
31	n	603	CLA	C3A-C2A-CAA-CBA
31	g	611	CLA	C3A-C2A-CAA-CBA
31	g	612	CLA	C3A-C2A-CAA-CBA
31	r	610	CLA	C3A-C2A-CAA-CBA
31	y	603	CLA	C3A-C2A-CAA-CBA
31	C1	507	CLA	C3A-C2A-CAA-CBA
31	C1	512	CLA	C3A-C2A-CAA-CBA
31	D1	402	CLA	C3A-C2A-CAA-CBA
31	N1	603	CLA	C3A-C2A-CAA-CBA
31	N1	613	CLA	C3A-C2A-CAA-CBA
31	G1	603	CLA	C3A-C2A-CAA-CBA
31	Y1	603	CLA	C3A-C2A-CAA-CBA
31	b1	603	CLA	C3A-C2A-CAA-CBA
31	c1	507	CLA	C3A-C2A-CAA-CBA
31	c1	511	CLA	C3A-C2A-CAA-CBA
31	c1	512	CLA	C3A-C2A-CAA-CBA
31	c1	513	CLA	C3A-C2A-CAA-CBA
31	n1	603	CLA	C3A-C2A-CAA-CBA
31	n1	610	CLA	C3A-C2A-CAA-CBA
31	n1	613	CLA	C3A-C2A-CAA-CBA
31	n1	614	CLA	C3A-C2A-CAA-CBA
31	s1	605	CLA	C3A-C2A-CAA-CBA
31	y1	603	CLA	C3A-C2A-CAA-CBA
32	a1	409	PHO	C3A-C2A-CAA-CBA
47	G	607	CHL	C3A-C2A-CAA-CBA
47	Y	606	CHL	C3A-C2A-CAA-CBA
47	n	609	CHL	C3A-C2A-CAA-CBA
47	g	607	CHL	C3A-C2A-CAA-CBA
47	y	605	CHL	C3A-C2A-CAA-CBA
47	y	606	CHL	C3A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	N1	607	CHL	C3A-C2A-CAA-CBA
47	g1	605	CHL	C3A-C2A-CAA-CBA
47	g1	607	CHL	C3A-C2A-CAA-CBA
31	G	603	CLA	C8-C10-C11-C12
33	b1	619	BCR	C19-C20-C21-C22
48	n1	621	LUT	C29-C30-C31-C32
48	g1	621	LUT	C29-C30-C31-C32
35	h1	102	LMG	C11-C12-C13-C14
38	C	524	DGA	CA5-CA6-CA7-CA8
38	C	524	DGA	CAB-CBB-CCB-CDB
38	B1	625	DGA	CA6-CA7-CA8-CA9
40	c1	518	DGD	C3A-C4A-C5A-C6A
41	L	101	LHG	C11-C12-C13-C14
41	D1	409	LHG	C28-C29-C30-C31
41	G1	624	LHG	C13-C14-C15-C16
41	d1	408	LHG	C30-C31-C32-C33
41	d1	408	LHG	C32-C33-C34-C35
41	y1	624	LHG	C15-C16-C17-C18
52	B1	624	3PH	C29-C2A-C2B-C2C
52	t1	101	3PH	C29-C2A-C2B-C2C
31	Y	611	CLA	O1D-CGD-O2D-CED
31	c1	506	CLA	O1D-CGD-O2D-CED
31	C1	510	CLA	O1A-CGA-O2A-C1
31	c1	510	CLA	O1A-CGA-O2A-C1
31	g1	610	CLA	O1A-CGA-O2A-C1
31	G	602	CLA	C16-C17-C18-C20
31	G	613	CLA	C16-C17-C18-C20
31	R	608	CLA	C11-C12-C13-C14
31	c	504	CLA	C16-C17-C18-C19
31	c	507	CLA	C16-C17-C18-C19
31	c	513	CLA	C16-C17-C18-C20
31	n	604	CLA	C16-C17-C18-C19
31	B1	609	CLA	C16-C17-C18-C20
31	B1	611	CLA	C16-C17-C18-C20
31	C1	501	CLA	C16-C17-C18-C20
31	G1	602	CLA	C16-C17-C18-C19
31	Y1	613	CLA	C16-C17-C18-C19
31	c1	507	CLA	C16-C17-C18-C20
31	r1	608	CLA	C11-C12-C13-C14
31	y1	613	CLA	C16-C17-C18-C19
31	y1	613	CLA	C16-C17-C18-C20
47	s1	608	CHL	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	A	412	SQD	C14-C15-C16-C17
40	c1	519	DGD	C3A-C4A-C5A-C6A
41	D	409	LHG	C29-C30-C31-C32
41	d	409	LHG	C28-C29-C30-C31
41	s	624	LHG	C26-C27-C28-C29
41	C1	525	LHG	C11-C12-C13-C14
41	C1	525	LHG	C13-C14-C15-C16
41	D1	408	LHG	C25-C26-C27-C28
41	Y1	624	LHG	C11-C10-C9-C8
41	Y1	624	LHG	C28-C29-C30-C31
41	d1	408	LHG	C26-C27-C28-C29
52	S1	626	3PH	C29-C2A-C2B-C2C
54	i1	101	4RF	C27-C28-C29-C30
54	i1	101	4RF	C44-C45-C46-C47
31	B	603	CLA	C13-C15-C16-C17
35	B1	622	LMG	C7-C8-C9-O8
38	j1	101	DGA	OG1-CG1-CG2-CG3
41	d	408	LHG	C4-C5-C6-O8
34	M1	101	SQD	C11-C10-C9-C8
35	C	521	LMG	C15-C16-C17-C18
38	B	625	DGA	CA4-CA5-CA6-CA7
41	L1	101	LHG	C26-C27-C28-C29
41	n1	624	LHG	C25-C26-C27-C28
41	n1	624	LHG	C28-C29-C30-C31
41	y1	624	LHG	C11-C12-C13-C14
52	S	626	3PH	C37-C38-C39-C3A
54	K1	101	4RF	C31-C32-C33-C34
50	r1	622	NEX	C14-C15-C35-C34
31	d	402	CLA	C3-C5-C6-C7
31	y1	613	CLA	C3-C5-C6-C7
47	n	601	CHL	C3-C5-C6-C7
41	s	624	LHG	C31-C32-C33-C34
41	L1	101	LHG	C11-C10-C9-C8
31	s	604	CLA	C5-C6-C7-C8
31	B1	603	CLA	C15-C16-C17-C18
31	N	613	CLA	C4-C3-C5-C6
31	B1	612	CLA	C4-C3-C5-C6
31	N1	604	CLA	C4-C3-C5-C6
31	c1	506	CLA	C4-C3-C5-C6
32	a	408	PHO	C4-C3-C5-C6
44	D	405	PL9	C30-C29-C31-C32
47	Y1	607	CHL	C4-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N	613	CLA	C2-C3-C5-C6
31	N1	613	CLA	C2-C3-C5-C6
31	c1	506	CLA	C2-C3-C5-C6
32	a	408	PHO	C2-C3-C5-C6
47	n1	605	CHL	C2-C3-C5-C6
35	a	413	LMG	C11-C10-O7-C8
38	c1	524	DGA	CB2-CB1-OG2-CG2
41	C1	525	LHG	C8-C7-O7-C5
41	D1	408	LHG	C8-C7-O7-C5
54	k1	101	4RF	C24-C22-O21-C20
41	N	624	LHG	C31-C32-C33-C34
41	C1	525	LHG	C24-C25-C26-C27
41	n1	624	LHG	C11-C12-C13-C14
52	B1	624	3PH	C3D-C3E-C3F-C3G
53	y	625	SPH	C11-C10-C9-C8
47	n	607	CHL	C2A-CAA-CBA-CGA
41	D	409	LHG	O1-C1-C2-O2
41	L	101	LHG	O1-C1-C2-O2
41	S	624	LHG	O1-C1-C2-O2
41	d	409	LHG	O1-C1-C2-O2
41	l	101	LHG	O1-C1-C2-O2
41	y	624	LHG	O1-C1-C2-O2
41	C1	525	LHG	O1-C1-C2-O2
41	D1	408	LHG	O1-C1-C2-O2
41	L1	101	LHG	O1-C1-C2-O2
41	N1	624	LHG	O1-C1-C2-O2
41	G1	624	LHG	O1-C1-C2-O2
41	S1	624	LHG	O1-C1-C2-O2
41	d1	409	LHG	O1-C1-C2-O2
41	s1	624	LHG	O1-C1-C2-O2
41	y1	624	LHG	O1-C1-C2-O2
31	C	512	CLA	C8-C10-C11-C12
31	b1	608	CLA	C10-C11-C12-C13
34	B	621	SQD	C13-C14-C15-C16
34	b	621	SQD	C32-C33-C34-C35
41	Y	624	LHG	C11-C10-C9-C8
41	c	625	LHG	C28-C29-C30-C31
41	l	101	LHG	C28-C29-C30-C31
41	l	101	LHG	C33-C34-C35-C36
41	g	624	LHG	C13-C14-C15-C16
41	y	624	LHG	C16-C17-C18-C19
41	y	624	LHG	C28-C29-C30-C31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	C1	525	LHG	C9-C10-C11-C12
41	G1	624	LHG	C28-C29-C30-C31
54	k1	101	4RF	C27-C28-C29-C30
55	R1	625	LMT	C5-C6-C7-C8
31	R	604	CLA	O1A-CGA-O2A-C1
31	g1	603	CLA	O1A-CGA-O2A-C1
35	J	101	LMG	C28-C29-C30-C31
52	i	101	3PH	C21-C22-C23-C24
31	B	617	CLA	C16-C17-C18-C20
31	g	602	CLA	C16-C17-C18-C19
31	R1	608	CLA	C11-C12-C13-C15
38	C1	524	DGA	CA6-CA7-CA8-CA9
41	D1	408	LHG	C11-C12-C13-C14
52	B1	624	3PH	C2A-C2B-C2C-C2D
54	I1	102	4RF	C09-C10-C11-C12
31	B	603	CLA	C10-C11-C12-C13
31	C	503	CLA	C13-C15-C16-C17
31	C	504	CLA	C10-C11-C12-C13
34	A1	412	SQD	C34-C35-C36-C37
34	b1	626	SQD	C11-C12-C13-C14
35	C	521	LMG	C16-C17-C18-C19
41	L1	101	LHG	C11-C12-C13-C14
31	C1	512	CLA	C3-C5-C6-C7
31	N	614	CLA	CBA-CGA-O2A-C1
38	B	625	DGA	CB9-CAB-CBB-CCB
38	B1	625	DGA	CB9-CAB-CBB-CCB
38	c1	524	DGA	CB2-CB3-CB4-CB5
41	g	624	LHG	C11-C12-C13-C14
41	D1	409	LHG	C34-C35-C36-C37
53	y1	625	SPH	C11-C12-C13-C14
31	Y	602	CLA	O1A-CGA-O2A-C1
31	B1	606	CLA	O1A-CGA-O2A-C1
51	S	625	LPX	O7-C6-O6-C5
40	c	518	DGD	C1B-C2B-C3B-C4B
40	C1	518	DGD	C1B-C2B-C3B-C4B
41	D1	408	LHG	C23-C24-C25-C26
31	b	605	CLA	C10-C11-C12-C13
31	c	509	CLA	C13-C15-C16-C17
31	c	512	CLA	C5-C6-C7-C8
34	B	621	SQD	C32-C33-C34-C35
34	a	412	SQD	C28-C29-C30-C31
41	D	408	LHG	C30-C31-C32-C33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	D	409	LHG	C28-C29-C30-C31
41	y1	624	LHG	C34-C35-C36-C37
35	a	413	LMG	O9-C10-O7-C8
38	c1	524	DGA	OB1-CB1-OG2-CG2
41	Y	624	LHG	O9-C7-O7-C5
41	d	410	LHG	O9-C7-O7-C5
31	B	603	CLA	C2-C1-O2A-CGA
31	B	607	CLA	C2-C1-O2A-CGA
31	B	615	CLA	C2-C1-O2A-CGA
31	C	502	CLA	C2-C1-O2A-CGA
31	C	503	CLA	C2-C1-O2A-CGA
31	N	613	CLA	C2-C1-O2A-CGA
31	N	614	CLA	C2-C1-O2A-CGA
31	G	604	CLA	C2-C1-O2A-CGA
31	R	604	CLA	C2-C1-O2A-CGA
31	S	603	CLA	C2-C1-O2A-CGA
31	S	609	CLA	C2-C1-O2A-CGA
31	S	614	CLA	C2-C1-O2A-CGA
31	a	407	CLA	C2-C1-O2A-CGA
31	b	603	CLA	C2-C1-O2A-CGA
31	b	607	CLA	C2-C1-O2A-CGA
31	b	611	CLA	C2-C1-O2A-CGA
31	g	614	CLA	C2-C1-O2A-CGA
31	r	602	CLA	C2-C1-O2A-CGA
31	s	617	CLA	C2-C1-O2A-CGA
31	y	603	CLA	C2-C1-O2A-CGA
31	B1	611	CLA	C2-C1-O2A-CGA
31	B1	616	CLA	C2-C1-O2A-CGA
31	B1	617	CLA	C2-C1-O2A-CGA
31	C1	507	CLA	C2-C1-O2A-CGA
31	C1	511	CLA	C2-C1-O2A-CGA
31	G1	611	CLA	C2-C1-O2A-CGA
31	G1	613	CLA	C2-C1-O2A-CGA
31	R1	612	CLA	C2-C1-O2A-CGA
31	S1	614	CLA	C2-C1-O2A-CGA
31	a1	405	CLA	C2-C1-O2A-CGA
31	c1	503	CLA	C2-C1-O2A-CGA
31	n1	603	CLA	C2-C1-O2A-CGA
31	g1	611	CLA	C2-C1-O2A-CGA
31	g1	613	CLA	C2-C1-O2A-CGA
31	r1	612	CLA	C2-C1-O2A-CGA
31	s1	614	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	y1	604	CLA	C2-C1-O2A-CGA
44	D	405	PL9	C32-C33-C34-C36
38	J1	101	DGA	CA4-CA5-CA6-CA7
38	j1	101	DGA	CA4-CA5-CA6-CA7
41	d	408	LHG	C26-C27-C28-C29
41	d	409	LHG	C26-C27-C28-C29
41	n	624	LHG	C28-C29-C30-C31
41	g	624	LHG	C28-C29-C30-C31
41	s	624	LHG	C9-C10-C11-C12
41	C1	525	LHG	C26-C27-C28-C29
41	S1	624	LHG	C29-C30-C31-C32
41	d1	408	LHG	C29-C30-C31-C32
52	b1	624	3PH	C28-C29-C2A-C2B
52	t1	101	3PH	C2A-C2B-C2C-C2D
52	s1	626	3PH	C24-C25-C26-C27
53	a1	414	SPH	C6-C7-C8-C9
53	y1	625	SPH	C6-C7-C8-C9
31	C	501	CLA	C13-C15-C16-C17
31	C	503	CLA	C10-C11-C12-C13
31	N	613	CLA	C5-C6-C7-C8
31	Y	613	CLA	C15-C16-C17-C18
31	B1	604	CLA	C5-C6-C7-C8
31	R1	603	CLA	C8-C10-C11-C12
31	y1	612	CLA	C13-C15-C16-C17
47	n	607	CHL	C8-C10-C11-C12
41	D1	410	LHG	C2-C3-O3-P
31	G1	603	CLA	O1A-CGA-O2A-C1
41	d	410	LHG	O10-C23-O8-C6
51	s1	625	LPX	O7-C6-O6-C5
35	D	411	LMG	C29-C30-C31-C32
35	d1	411	LMG	C19-C20-C21-C22
41	N	624	LHG	C26-C27-C28-C29
41	S	624	LHG	C12-C13-C14-C15
41	d	408	LHG	C11-C12-C13-C14
41	Y1	624	LHG	C13-C14-C15-C16
41	c1	525	LHG	C11-C10-C9-C8
41	g1	624	LHG	C15-C16-C17-C18
53	a1	414	SPH	C11-C12-C13-C14
34	C1	526	SQD	C7-C8-C9-C10
41	g1	624	LHG	C23-C24-C25-C26
31	C	505	CLA	C3-C5-C6-C7
33	A	411	BCR	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	B	618	BCR	C23-C24-C25-C30
33	C	514	BCR	C1-C6-C7-C8
33	C	514	BCR	C5-C6-C7-C8
33	C	515	BCR	C23-C24-C25-C26
33	C	515	BCR	C23-C24-C25-C30
33	C	516	BCR	C23-C24-C25-C26
33	C	516	BCR	C23-C24-C25-C30
33	C	517	BCR	C23-C24-C25-C26
33	D	404	BCR	C1-C6-C7-C8
33	D	404	BCR	C5-C6-C7-C8
33	D	404	BCR	C23-C24-C25-C26
33	a	411	BCR	C23-C24-C25-C26
33	b	618	BCR	C1-C6-C7-C8
33	b	618	BCR	C5-C6-C7-C8
33	c	514	BCR	C1-C6-C7-C8
33	c	514	BCR	C5-C6-C7-C8
33	c	514	BCR	C23-C24-C25-C26
33	c	516	BCR	C5-C6-C7-C8
33	c	517	BCR	C23-C24-C25-C26
33	c	517	BCR	C23-C24-C25-C30
33	d	404	BCR	C1-C6-C7-C8
33	d	404	BCR	C5-C6-C7-C8
33	A1	411	BCR	C23-C24-C25-C26
33	A1	411	BCR	C23-C24-C25-C30
33	C1	514	BCR	C1-C6-C7-C8
33	C1	514	BCR	C5-C6-C7-C8
33	C1	514	BCR	C23-C24-C25-C26
33	C1	514	BCR	C23-C24-C25-C30
33	C1	516	BCR	C23-C24-C25-C26
33	C1	516	BCR	C23-C24-C25-C30
33	C1	517	BCR	C23-C24-C25-C30
33	D1	404	BCR	C1-C6-C7-C8
33	D1	404	BCR	C5-C6-C7-C8
33	a1	411	BCR	C23-C24-C25-C26
33	a1	411	BCR	C23-C24-C25-C30
33	c1	514	BCR	C1-C6-C7-C8
33	c1	514	BCR	C5-C6-C7-C8
33	c1	514	BCR	C23-C24-C25-C26
33	c1	515	BCR	C23-C24-C25-C26
33	c1	516	BCR	C1-C6-C7-C8
33	c1	516	BCR	C5-C6-C7-C8
33	d1	404	BCR	C1-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	d1	404	BCR	C5-C6-C7-C8
37	B1	620	C7Z	C1-C6-C7-C8
37	B1	620	C7Z	C21-C26-C27-C28
37	b1	620	C7Z	C1-C6-C7-C8
37	b1	620	C7Z	C25-C26-C27-C28
46	H	101	RRX	C23-C24-C25-C30
46	H	101	RRX	C23-C24-C25-C26
48	N1	620	LUT	C5-C6-C7-C8
34	a	412	SQD	C10-C11-C12-C13
38	c	524	DGA	CDA-CEA-CFA-CGA
41	D1	409	LHG	C26-C27-C28-C29
41	L1	101	LHG	C31-C32-C33-C34
54	K1	101	4RF	C29-C30-C31-C32
40	C1	520	DGD	C2A-C1A-O1G-C1G
31	A	410	CLA	C8-C10-C11-C12
31	C	501	CLA	C5-C6-C7-C8
31	C	502	CLA	C10-C11-C12-C13
31	C	510	CLA	C5-C6-C7-C8
31	D	402	CLA	C15-C16-C17-C18
31	S	603	CLA	C5-C6-C7-C8
31	S	603	CLA	C15-C16-C17-C18
31	Y	602	CLA	C8-C10-C11-C12
31	c	508	CLA	C10-C11-C12-C13
31	g	602	CLA	C5-C6-C7-C8
31	r	612	CLA	C8-C10-C11-C12
31	y	614	CLA	C5-C6-C7-C8
31	B1	617	CLA	C15-C16-C17-C18
31	C1	508	CLA	C8-C10-C11-C12
31	N1	613	CLA	C15-C16-C17-C18
31	G1	603	CLA	C5-C6-C7-C8
31	S1	603	CLA	C5-C6-C7-C8
31	b1	610	CLA	C8-C10-C11-C12
31	d1	403	CLA	C10-C11-C12-C13
31	s1	603	CLA	C8-C10-C11-C12
31	s1	611	CLA	C10-C11-C12-C13
31	y1	603	CLA	C5-C6-C7-C8
41	d1	410	LHG	C8-C7-O7-C5
34	c	626	SQD	C13-C14-C15-C16
35	a	413	LMG	C16-C17-C18-C19
38	B1	625	DGA	CBA-CCA-CDA-CEA
41	N	624	LHG	C16-C17-C18-C19
41	c	625	LHG	C11-C10-C9-C8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	D1	409	LHG	C25-C26-C27-C28
42	c1	527	LMK	C17-C18-C19-C20
54	k1	101	4RF	C24-C25-C26-C27
31	Y1	614	CLA	O1A-CGA-O2A-C1
31	S	602	CLA	CBD-CGD-O2D-CED
41	C1	525	LHG	C7-C8-C9-C10
35	c1	521	LMG	C36-C37-C38-C39
38	c1	524	DGA	CAB-CBB-CCB-CDB
41	c	625	LHG	C31-C32-C33-C34
41	n	624	LHG	C31-C32-C33-C34
51	s	625	LPX	C7-C8-C9-C10
54	i1	101	4RF	C25-C26-C27-C28
44	d	405	PL9	C47-C48-C49-C50
31	B	605	CLA	C8-C10-C11-C12
31	a	405	CLA	C10-C11-C12-C13
31	c	510	CLA	C13-C15-C16-C17
31	c1	510	CLA	C5-C6-C7-C8
31	g1	610	CLA	C8-C10-C11-C12
35	j	101	LMG	C31-C32-C33-C34
41	S	624	LHG	C11-C12-C13-C14
41	l	101	LHG	C31-C32-C33-C34
54	K1	101	4RF	C32-C33-C34-C35
31	b	602	CLA	C4-C3-C5-C6
31	s	602	CLA	C4-C3-C5-C6
31	s	611	CLA	C4-C3-C5-C6
31	b1	612	CLA	C4-C3-C5-C6
44	D	405	PL9	C15-C14-C16-C17
47	y	607	CHL	C4-C3-C5-C6
31	A	405	CLA	C11-C12-C13-C15
31	B	602	CLA	C6-C7-C8-C10
31	B	606	CLA	C11-C12-C13-C15
31	C	506	CLA	C11-C12-C13-C15
31	C	510	CLA	C2-C3-C5-C6
31	C	512	CLA	C11-C12-C13-C15
31	N	604	CLA	C6-C7-C8-C10
31	N	613	CLA	C12-C13-C15-C16
31	Y	602	CLA	C12-C13-C15-C16
31	Y	604	CLA	C12-C13-C15-C16
31	Y	610	CLA	C11-C12-C13-C15
31	Y	611	CLA	C11-C10-C8-C7
31	b	602	CLA	C6-C7-C8-C10
31	b	606	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	505	CLA	C11-C10-C8-C7
31	n	602	CLA	C11-C10-C8-C7
31	n	604	CLA	C6-C7-C8-C10
31	r	610	CLA	C11-C10-C8-C7
31	s	610	CLA	C11-C12-C13-C15
31	s	611	CLA	C6-C7-C8-C10
31	y	602	CLA	C11-C12-C13-C15
31	y	604	CLA	C12-C13-C15-C16
31	y	613	CLA	C11-C12-C13-C15
31	B1	607	CLA	C11-C12-C13-C15
31	B1	611	CLA	C11-C10-C8-C7
31	B1	612	CLA	C2-C3-C5-C6
31	B1	613	CLA	C12-C13-C15-C16
31	B1	615	CLA	C6-C7-C8-C10
31	B1	617	CLA	C11-C12-C13-C15
31	C1	508	CLA	C11-C12-C13-C15
31	C1	512	CLA	C12-C13-C15-C16
31	N1	603	CLA	C2-C3-C5-C6
31	N1	604	CLA	C6-C7-C8-C10
31	Y1	604	CLA	C11-C10-C8-C7
31	b1	605	CLA	C6-C7-C8-C10
31	b1	613	CLA	C12-C13-C15-C16
31	c1	511	CLA	C6-C7-C8-C10
31	n1	602	CLA	C12-C13-C15-C16
31	n1	610	CLA	C6-C7-C8-C10
31	g1	613	CLA	C12-C13-C15-C16
31	r1	608	CLA	C11-C10-C8-C7
31	y1	602	CLA	C11-C12-C13-C15
44	D	405	PL9	C13-C14-C16-C17
44	d1	405	PL9	C18-C19-C21-C22
44	d1	405	PL9	C38-C39-C41-C42
47	y	607	CHL	C2-C3-C5-C6
47	y	609	CHL	C11-C12-C13-C15
47	Y1	607	CHL	C2-C3-C5-C6
47	g1	601	CHL	C11-C12-C13-C15
47	g1	601	CHL	C12-C13-C15-C16
47	g1	607	CHL	C11-C10-C8-C7
47	y1	606	CHL	C6-C7-C8-C10
47	y1	607	CHL	C12-C13-C15-C16
31	b	615	CLA	C3-C5-C6-C7
31	B1	615	CLA	C3-C5-C6-C7
31	S1	614	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b1	615	CLA	C3-C5-C6-C7
31	N	614	CLA	O1A-CGA-O2A-C1
41	C	525	LHG	O10-C23-O8-C6
41	C1	525	LHG	O10-C23-O8-C6
41	d1	410	LHG	O10-C23-O8-C6
54	K1	101	4RF	O17-C16-O18-C19
54	i1	101	4RF	O42-C41-O40-C39
41	D	410	LHG	C24-C25-C26-C27
52	s1	626	3PH	C25-C26-C27-C28
31	B	603	CLA	C8-C10-C11-C12
31	s	602	CLA	C8-C10-C11-C12
31	b1	614	CLA	C8-C10-C11-C12
31	c1	501	CLA	C13-C15-C16-C17
31	c1	506	CLA	C13-C15-C16-C17
33	b	618	BCR	C9-C10-C11-C12
33	c	514	BCR	C13-C14-C15-C16
33	c	517	BCR	C9-C10-C11-C12
33	d1	404	BCR	C19-C20-C21-C22
46	H	101	RRX	C15-C16-C17-C18
48	n	620	LUT	C29-C30-C31-C32
31	B	616	CLA	C16-C17-C18-C20
31	S	609	CLA	C11-C12-C13-C15
31	S1	602	CLA	C11-C12-C13-C15
31	Y1	614	CLA	C16-C17-C18-C20
31	g1	602	CLA	C16-C17-C18-C19
31	r1	610	CLA	C11-C12-C13-C15
34	B1	626	SQD	O49-C7-O47-C45
35	H1	102	LMG	O9-C10-O7-C8
54	k1	101	4RF	O23-C22-O21-C20
38	b	623	DGA	CB1-CB2-CB3-CB4
40	C	518	DGD	C1B-C2B-C3B-C4B
41	d	409	LHG	C23-C24-C25-C26
41	l	101	LHG	C23-C24-C25-C26
41	y1	624	LHG	C23-C24-C25-C26
31	S	610	CLA	CBA-CGA-O2A-C1
31	c	508	CLA	CBA-CGA-O2A-C1
31	C1	502	CLA	CBA-CGA-O2A-C1
31	C1	508	CLA	CBA-CGA-O2A-C1
40	c1	518	DGD	C2A-C1A-O1G-C1G
52	s1	626	3PH	C32-C31-O31-C3
54	K1	101	4RF	C43-C41-O40-C39
34	B1	621	SQD	C26-C27-C28-C29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	B1	626	SQD	C30-C31-C32-C33
41	L1	101	LHG	C10-C11-C12-C13
41	Y1	624	LHG	C16-C17-C18-C19
52	B1	624	3PH	C3A-C3B-C3C-C3D
54	I1	102	4RF	C51-C52-C53-C54
57	y1	627	PTY	C31-C30-O4-C1
31	B	604	CLA	C2A-CAA-CBA-CGA
31	C	501	CLA	C2A-CAA-CBA-CGA
31	N	604	CLA	C2A-CAA-CBA-CGA
31	G	604	CLA	C2A-CAA-CBA-CGA
31	G	610	CLA	C2A-CAA-CBA-CGA
31	R	613	CLA	C2A-CAA-CBA-CGA
31	Y	610	CLA	C2A-CAA-CBA-CGA
31	b	604	CLA	C2A-CAA-CBA-CGA
31	r	604	CLA	C2A-CAA-CBA-CGA
31	B1	604	CLA	C2A-CAA-CBA-CGA
31	S1	603	CLA	C2A-CAA-CBA-CGA
31	Y1	608	CLA	C2A-CAA-CBA-CGA
31	r1	602	CLA	C2A-CAA-CBA-CGA
47	N	606	CHL	C2A-CAA-CBA-CGA
47	r	607	CHL	C2A-CAA-CBA-CGA
47	g1	607	CHL	C2A-CAA-CBA-CGA
31	B	606	CLA	C5-C6-C7-C8
31	G	603	CLA	C10-C11-C12-C13
31	c	511	CLA	C5-C6-C7-C8
31	y	613	CLA	C15-C16-C17-C18
31	C1	503	CLA	C5-C6-C7-C8
31	R1	602	CLA	C8-C10-C11-C12
31	c1	508	CLA	C15-C16-C17-C18
31	y1	613	CLA	C10-C11-C12-C13
35	C1	523	LMG	C16-C17-C18-C19
41	Y	624	LHG	C9-C10-C11-C12
41	d1	408	LHG	C33-C34-C35-C36
41	s1	624	LHG	C31-C32-C33-C34
42	c1	527	LMK	C11-C12-C13-C14
54	k1	101	4RF	C11-C12-C13-C14
55	r1	625	LMT	C9-C10-C11-C12
31	c	505	CLA	CBD-CGD-O2D-CED
41	n	624	LHG	C14-C15-C16-C17
55	r1	625	LMT	C4-C5-C6-C7
57	y1	626	PTY	C31-C32-C33-C34
31	n	603	CLA	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B1	615	CLA	C13-C15-C16-C17
34	b1	626	SQD	C11-C10-C9-C8
38	B1	625	DGA	CCA-CDA-CEA-CFA
40	C1	518	DGD	C5B-C6B-C7B-C8B
41	D	408	LHG	C12-C13-C14-C15
41	D	409	LHG	C31-C32-C33-C34
41	D	409	LHG	C34-C35-C36-C37
41	L	101	LHG	C33-C34-C35-C36
41	n	624	LHG	C15-C16-C17-C18
41	d1	408	LHG	C11-C10-C9-C8
41	y1	624	LHG	C33-C34-C35-C36
52	b1	624	3PH	C32-C33-C34-C35
44	D	405	PL9	C37-C38-C39-C40
44	d	405	PL9	C12-C13-C14-C15
31	G1	603	CLA	C3-C5-C6-C7
34	c	626	SQD	C18-C19-C20-C21
38	c	524	DGA	CB9-CAB-CBB-CCB
40	C1	519	DGD	C4A-C5A-C6A-C7A
41	D	410	LHG	C11-C10-C9-C8
54	i1	101	4RF	C32-C33-C34-C35
31	c	509	CLA	CBA-CGA-O2A-C1
31	y	602	CLA	CBA-CGA-O2A-C1
40	C1	519	DGD	C2A-C1A-O1G-C1G
40	c1	520	DGD	C4E-C5E-C6E-O5E
40	C	518	DGD	O6E-C1E-O5D-C6D
40	C1	519	DGD	O6D-C1D-O3G-C3G
31	C	508	CLA	C10-C11-C12-C13
31	b	607	CLA	C5-C6-C7-C8
31	G1	611	CLA	C5-C6-C7-C8
31	c1	504	CLA	C8-C10-C11-C12
35	J	101	LMG	C31-C32-C33-C34
35	c	521	LMG	C29-C30-C31-C32
35	b1	622	LMG	C31-C32-C33-C34
38	b1	625	DGA	CB6-CB7-CB8-CB9
41	D	408	LHG	C26-C27-C28-C29
41	L	101	LHG	C31-C32-C33-C34
41	d	410	LHG	C11-C10-C9-C8
41	G1	624	LHG	C24-C25-C26-C27
54	K1	101	4RF	C34-C35-C36-C37
57	y1	626	PTY	C11-C12-C13-C14
41	s	624	LHG	C23-C24-C25-C26
41	D1	409	LHG	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	A	412	SQD	C8-C7-O47-C45
34	c	626	SQD	C8-C7-O47-C45
34	B1	626	SQD	C8-C7-O47-C45
35	h	102	LMG	C11-C10-O7-C8
35	H1	102	LMG	C11-C10-O7-C8
35	c1	523	LMG	C11-C10-O7-C8
40	C1	519	DGD	C2B-C1B-O2G-C2G
41	D	410	LHG	C8-C7-O7-C5
41	c	625	LHG	C8-C7-O7-C5
41	y	624	LHG	C8-C7-O7-C5
52	i	101	3PH	C22-C21-O21-C2
52	B1	624	3PH	C22-C21-O21-C2
50	g	623	NEX	C30-C31-C32-C33
34	B1	626	SQD	C26-C27-C28-C29
41	S	624	LHG	C9-C10-C11-C12
41	D1	409	LHG	C11-C10-C9-C8
41	y1	624	LHG	C11-C10-C9-C8
52	T1	101	3PH	C29-C2A-C2B-C2C
52	t1	101	3PH	C26-C27-C28-C29
53	a1	414	SPH	C14-C15-C16-C17
54	K1	101	4RF	C43-C44-C45-C46
54	i1	101	4RF	C09-C10-C11-C12
45	f	101	HEM	C4B-C3B-CAB-CBB
31	A	405	CLA	C5-C6-C7-C8
31	C	510	CLA	C15-C16-C17-C18
31	Y	610	CLA	C8-C10-C11-C12
31	C1	505	CLA	C15-C16-C17-C18
31	C1	512	CLA	C5-C6-C7-C8
31	S1	609	CLA	C10-C11-C12-C13
31	r1	612	CLA	C5-C6-C7-C8
41	D1	410	LHG	O10-C23-O8-C6
34	c	626	SQD	C16-C17-C18-C19
34	A1	412	SQD	C11-C12-C13-C14
35	D	411	LMG	C11-C12-C13-C14
38	c1	524	DGA	CA5-CA6-CA7-CA8
41	C	525	LHG	C13-C14-C15-C16
35	h	102	LMG	O9-C10-O7-C8
42	C	527	LMK	C2-C3-C4-O2
34	c	626	SQD	C11-C10-C9-C8
34	b1	621	SQD	C25-C26-C27-C28
54	k1	101	4RF	C05-C06-C07-C08
56	R1	626	ERG	C21-C20-C22-C23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
56	r1	626	ERG	C21-C20-C22-C23
34	a	412	SQD	C2-C1-O6-C44
40	C	518	DGD	C2E-C1E-O5D-C6D
40	B1	623	DGD	C2D-C1D-O3G-C3G
40	C1	519	DGD	C2D-C1D-O3G-C3G
34	B1	626	SQD	O47-C45-C46-O48
35	a1	413	LMG	O1-C7-C8-O7
40	c1	519	DGD	O1G-C1G-C2G-O2G
41	d	410	LHG	O7-C5-C6-O8
40	C1	519	DGD	CCB-CDB-CEB-CFB
41	G	630	LHG	C12-C13-C14-C15
54	i1	101	4RF	C26-C27-C28-C29
31	b1	605	CLA	C16-C17-C18-C20
31	s1	604	CLA	C6-C7-C8-C9
41	D1	408	LHG	C11-C10-C9-C8
35	h	102	LMG	O6-C5-C6-O5
31	B	617	CLA	C8-C10-C11-C12
31	G	603	CLA	C13-C15-C16-C17
31	Y	604	CLA	C10-C11-C12-C13
31	b	606	CLA	C5-C6-C7-C8
31	n	603	CLA	C10-C11-C12-C13
31	s	603	CLA	C5-C6-C7-C8
31	b1	608	CLA	C5-C6-C7-C8
31	b1	615	CLA	C8-C10-C11-C12
31	c1	510	CLA	C13-C15-C16-C17
53	A1	414	SPH	C5-C6-C7-C8
31	C	510	CLA	C4-C3-C5-C6
31	N1	603	CLA	C4-C3-C5-C6
31	N1	613	CLA	C4-C3-C5-C6
31	n1	610	CLA	C4-C3-C5-C6
44	d	405	PL9	C15-C14-C16-C17
47	n1	605	CHL	C4-C3-C5-C6
41	N1	624	LHG	C23-C24-C25-C26
52	T1	101	3PH	C31-C32-C33-C34
52	t1	101	3PH	C31-C32-C33-C34
57	Y1	626	PTY	C30-C31-C32-C33
31	b	602	CLA	C2-C3-C5-C6
31	c	513	CLA	C2-C3-C5-C6
31	N1	604	CLA	C2-C3-C5-C6
31	b1	612	CLA	C2-C3-C5-C6
44	D	405	PL9	C4-C3-C7-C8
44	d	405	PL9	C4-C3-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
44	d1	405	PL9	C4-C3-C7-C8
35	d1	411	LMG	C12-C13-C14-C15
38	j1	101	DGA	CB7-CB8-CB9-CAB
40	c	518	DGD	C3A-C4A-C5A-C6A
41	D	410	LHG	C28-C29-C30-C31
52	s1	626	3PH	C35-C36-C37-C38
57	Y1	626	PTY	C39-C40-C41-C42
31	A	405	CLA	C11-C12-C13-C14
31	B	602	CLA	C6-C7-C8-C9
31	B	602	CLA	C11-C10-C8-C9
31	B	604	CLA	C6-C7-C8-C9
31	C	506	CLA	C11-C10-C8-C9
31	C	507	CLA	C11-C12-C13-C14
31	C	508	CLA	C11-C10-C8-C9
31	D	403	CLA	C14-C13-C15-C16
31	N	604	CLA	C6-C7-C8-C9
31	G	610	CLA	C11-C12-C13-C14
31	G	613	CLA	C6-C7-C8-C9
31	Y	604	CLA	C14-C13-C15-C16
31	Y	610	CLA	C11-C12-C13-C14
31	Y	613	CLA	C11-C12-C13-C14
31	b	616	CLA	C11-C12-C13-C14
31	c	513	CLA	C11-C12-C13-C14
31	n	603	CLA	C6-C7-C8-C9
31	n	603	CLA	C11-C12-C13-C14
31	n	604	CLA	C6-C7-C8-C9
31	n	613	CLA	C11-C12-C13-C14
31	g	602	CLA	C11-C12-C13-C14
31	s	610	CLA	C11-C10-C8-C9
31	y	602	CLA	C6-C7-C8-C9
31	y	604	CLA	C11-C12-C13-C14
31	y	604	CLA	C14-C13-C15-C16
31	B1	602	CLA	C11-C10-C8-C9
31	B1	604	CLA	C6-C7-C8-C9
31	B1	617	CLA	C11-C12-C13-C14
31	C1	508	CLA	C11-C12-C13-C14
31	C1	513	CLA	C6-C7-C8-C9
31	D1	403	CLA	C11-C10-C8-C9
31	N1	610	CLA	C11-C12-C13-C14
31	G1	603	CLA	C6-C7-C8-C9
31	S1	609	CLA	C6-C7-C8-C9
31	Y1	613	CLA	C11-C12-C13-C14

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b1	603	CLA	C6-C7-C8-C9
31	b1	607	CLA	C11-C12-C13-C14
31	b1	617	CLA	C6-C7-C8-C9
31	c1	510	CLA	C14-C13-C15-C16
31	c1	513	CLA	C6-C7-C8-C9
31	c1	513	CLA	C11-C12-C13-C14
31	n1	602	CLA	C14-C13-C15-C16
31	g1	603	CLA	C11-C12-C13-C14
31	g1	610	CLA	C11-C10-C8-C9
31	g1	611	CLA	C6-C7-C8-C9
31	g1	613	CLA	C14-C13-C15-C16
31	y1	602	CLA	C11-C12-C13-C14
31	y1	613	CLA	C11-C12-C13-C14
47	G1	601	CHL	C11-C12-C13-C14
47	G1	607	CHL	C14-C13-C15-C16
47	n1	605	CHL	C11-C10-C8-C9
47	g1	601	CHL	C11-C12-C13-C14
47	g1	607	CHL	C11-C10-C8-C9
40	b1	623	DGD	O6E-C5E-C6E-O5E
38	C1	524	DGA	CB9-CAB-CBB-CCB
41	c	625	LHG	C24-C25-C26-C27
31	Y	611	CLA	C3-C5-C6-C7
31	B	612	CLA	C2A-CAA-CBA-CGA
31	S	605	CLA	C2A-CAA-CBA-CGA
31	S	610	CLA	C2A-CAA-CBA-CGA
31	c	510	CLA	C2A-CAA-CBA-CGA
31	n	602	CLA	C2A-CAA-CBA-CGA
31	r	603	CLA	C2A-CAA-CBA-CGA
31	s	610	CLA	C2A-CAA-CBA-CGA
31	C1	505	CLA	C2A-CAA-CBA-CGA
31	N1	602	CLA	C2A-CAA-CBA-CGA
31	Y1	610	CLA	C2A-CAA-CBA-CGA
31	a1	406	CLA	C2A-CAA-CBA-CGA
32	a1	409	PHO	C2A-CAA-CBA-CGA
47	N	608	CHL	C2A-CAA-CBA-CGA
47	G1	607	CHL	C2A-CAA-CBA-CGA
38	B	625	DGA	CAA-CBA-CCA-CDA
41	d1	408	LHG	C28-C29-C30-C31
52	S	626	3PH	C29-C2A-C2B-C2C
40	c1	518	DGD	O6E-C5E-C6E-O5E
33	c	514	BCR	C37-C22-C23-C24
48	n	621	LUT	C31-C32-C33-C40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
48	s1	620	LUT	C31-C32-C33-C40
31	b	615	CLA	C15-C16-C17-C18
31	A1	410	CLA	C8-C10-C11-C12
31	S1	610	CLA	C13-C15-C16-C17
34	c1	526	SQD	C24-C25-C26-C27
41	G	630	LHG	C13-C14-C15-C16
52	t1	101	3PH	C2B-C2C-C2D-C2E
54	I1	102	4RF	C11-C12-C13-C14
54	I1	102	4RF	C44-C45-C46-C47
33	b	618	BCR	C17-C18-C19-C20
48	Y1	620	LUT	C27-C28-C29-C30
40	c1	518	DGD	O1A-C1A-O1G-C1G
31	A	407	CLA	C1A-C2A-CAA-CBA
31	A	410	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	C1A-C2A-CAA-CBA
31	B	604	CLA	C1A-C2A-CAA-CBA
31	B	606	CLA	C1A-C2A-CAA-CBA
31	B	607	CLA	C1A-C2A-CAA-CBA
31	C	501	CLA	C1A-C2A-CAA-CBA
31	C	503	CLA	C1A-C2A-CAA-CBA
31	C	511	CLA	C1A-C2A-CAA-CBA
31	N	603	CLA	C1A-C2A-CAA-CBA
31	G	603	CLA	C1A-C2A-CAA-CBA
31	G	610	CLA	C1A-C2A-CAA-CBA
31	G	611	CLA	C1A-C2A-CAA-CBA
31	G	614	CLA	C1A-C2A-CAA-CBA
31	R	608	CLA	C1A-C2A-CAA-CBA
31	R	613	CLA	C1A-C2A-CAA-CBA
31	S	609	CLA	C1A-C2A-CAA-CBA
31	S	610	CLA	C1A-C2A-CAA-CBA
31	Y	602	CLA	C1A-C2A-CAA-CBA
31	Y	603	CLA	C1A-C2A-CAA-CBA
31	Y	604	CLA	C1A-C2A-CAA-CBA
31	Y	610	CLA	C1A-C2A-CAA-CBA
31	a	405	CLA	C1A-C2A-CAA-CBA
31	a	407	CLA	C1A-C2A-CAA-CBA
31	b	602	CLA	C1A-C2A-CAA-CBA
31	b	604	CLA	C1A-C2A-CAA-CBA
31	b	605	CLA	C1A-C2A-CAA-CBA
31	b	606	CLA	C1A-C2A-CAA-CBA
31	b	610	CLA	C1A-C2A-CAA-CBA
31	c	503	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	504	CLA	C1A-C2A-CAA-CBA
31	c	511	CLA	C1A-C2A-CAA-CBA
31	n	602	CLA	C1A-C2A-CAA-CBA
31	g	603	CLA	C1A-C2A-CAA-CBA
31	g	610	CLA	C1A-C2A-CAA-CBA
31	g	611	CLA	C1A-C2A-CAA-CBA
31	r	613	CLA	C1A-C2A-CAA-CBA
31	s	609	CLA	C1A-C2A-CAA-CBA
31	s	617	CLA	C1A-C2A-CAA-CBA
31	y	602	CLA	C1A-C2A-CAA-CBA
31	y	603	CLA	C1A-C2A-CAA-CBA
31	y	604	CLA	C1A-C2A-CAA-CBA
31	y	608	CLA	C1A-C2A-CAA-CBA
31	y	610	CLA	C1A-C2A-CAA-CBA
31	y	611	CLA	C1A-C2A-CAA-CBA
31	A1	405	CLA	C1A-C2A-CAA-CBA
31	B1	604	CLA	C1A-C2A-CAA-CBA
31	B1	607	CLA	C1A-C2A-CAA-CBA
31	C1	501	CLA	C1A-C2A-CAA-CBA
31	C1	503	CLA	C1A-C2A-CAA-CBA
31	C1	507	CLA	C1A-C2A-CAA-CBA
31	C1	511	CLA	C1A-C2A-CAA-CBA
31	N1	602	CLA	C1A-C2A-CAA-CBA
31	N1	603	CLA	C1A-C2A-CAA-CBA
31	G1	603	CLA	C1A-C2A-CAA-CBA
31	G1	610	CLA	C1A-C2A-CAA-CBA
31	G1	611	CLA	C1A-C2A-CAA-CBA
31	G1	614	CLA	C1A-C2A-CAA-CBA
31	R1	602	CLA	C1A-C2A-CAA-CBA
31	R1	609	CLA	C1A-C2A-CAA-CBA
31	R1	610	CLA	C1A-C2A-CAA-CBA
31	S1	602	CLA	C1A-C2A-CAA-CBA
31	S1	604	CLA	C1A-C2A-CAA-CBA
31	S1	617	CLA	C1A-C2A-CAA-CBA
31	Y1	603	CLA	C1A-C2A-CAA-CBA
31	Y1	608	CLA	C1A-C2A-CAA-CBA
31	Y1	610	CLA	C1A-C2A-CAA-CBA
31	Y1	611	CLA	C1A-C2A-CAA-CBA
31	Y1	614	CLA	C1A-C2A-CAA-CBA
31	a1	405	CLA	C1A-C2A-CAA-CBA
31	a1	410	CLA	C1A-C2A-CAA-CBA
31	b1	604	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b1	606	CLA	C1A-C2A-CAA-CBA
31	b1	607	CLA	C1A-C2A-CAA-CBA
31	b1	610	CLA	C1A-C2A-CAA-CBA
31	c1	503	CLA	C1A-C2A-CAA-CBA
31	c1	507	CLA	C1A-C2A-CAA-CBA
31	c1	512	CLA	C1A-C2A-CAA-CBA
31	n1	602	CLA	C1A-C2A-CAA-CBA
31	n1	603	CLA	C1A-C2A-CAA-CBA
31	g1	603	CLA	C1A-C2A-CAA-CBA
31	g1	610	CLA	C1A-C2A-CAA-CBA
31	g1	611	CLA	C1A-C2A-CAA-CBA
31	r1	602	CLA	C1A-C2A-CAA-CBA
31	r1	609	CLA	C1A-C2A-CAA-CBA
31	r1	610	CLA	C1A-C2A-CAA-CBA
31	s1	602	CLA	C1A-C2A-CAA-CBA
31	s1	603	CLA	C1A-C2A-CAA-CBA
31	s1	604	CLA	C1A-C2A-CAA-CBA
31	s1	609	CLA	C1A-C2A-CAA-CBA
31	s1	617	CLA	C1A-C2A-CAA-CBA
31	y1	603	CLA	C1A-C2A-CAA-CBA
31	y1	611	CLA	C1A-C2A-CAA-CBA
31	y1	614	CLA	C1A-C2A-CAA-CBA
47	G	609	CHL	C1A-C2A-CAA-CBA
47	S	608	CHL	C1A-C2A-CAA-CBA
47	Y	606	CHL	C1A-C2A-CAA-CBA
47	Y	609	CHL	C1A-C2A-CAA-CBA
47	g	609	CHL	C1A-C2A-CAA-CBA
47	y	606	CHL	C1A-C2A-CAA-CBA
47	g1	601	CHL	C1A-C2A-CAA-CBA
47	g1	605	CHL	C1A-C2A-CAA-CBA
47	g1	609	CHL	C1A-C2A-CAA-CBA
31	C	507	CLA	C16-C17-C18-C19
31	G	603	CLA	C16-C17-C18-C20
31	S	613	CLA	C6-C7-C8-C9
31	y	611	CLA	C16-C17-C18-C20
31	B1	602	CLA	C16-C17-C18-C20
31	B1	611	CLA	C16-C17-C18-C19
31	G1	602	CLA	C16-C17-C18-C20
31	S1	603	CLA	C16-C17-C18-C20
31	S1	604	CLA	C6-C7-C8-C9
31	r1	610	CLA	C11-C12-C13-C14
31	y1	614	CLA	C16-C17-C18-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	S1	608	CHL	C11-C12-C13-C14
34	A	412	SQD	O49-C7-O47-C45
34	c	626	SQD	O49-C7-O47-C45
35	c1	523	LMG	O9-C10-O7-C8
40	C1	519	DGD	O1B-C1B-O2G-C2G
41	c	625	LHG	O9-C7-O7-C5
41	y	624	LHG	O9-C7-O7-C5
41	D1	408	LHG	O9-C7-O7-C5
52	i	101	3PH	O22-C21-O21-C2
38	C1	524	DGA	CB5-CB6-CB7-CB8
41	D	409	LHG	C26-C27-C28-C29
41	C1	525	LHG	C28-C29-C30-C31
41	s1	624	LHG	C12-C13-C14-C15
41	y1	624	LHG	C9-C10-C11-C12
54	k1	101	4RF	C47-C48-C49-C50
33	B	618	BCR	C9-C10-C11-C12
33	C	516	BCR	C15-C16-C17-C18
33	c	515	BCR	C19-C20-C21-C22
37	b1	620	C7Z	C9-C10-C11-C12
48	G	620	LUT	C29-C30-C31-C32
48	y	621	LUT	C29-C30-C31-C32
48	n1	621	LUT	C9-C10-C11-C12
48	g1	620	LUT	C29-C30-C31-C32
31	C	508	CLA	C8-C10-C11-C12
31	D	403	CLA	C5-C6-C7-C8
31	B1	611	CLA	C10-C11-C12-C13
31	C1	509	CLA	C15-C16-C17-C18
31	Y1	613	CLA	C8-C10-C11-C12
31	c1	512	CLA	C5-C6-C7-C8
31	g1	603	CLA	C10-C11-C12-C13
57	y1	626	PTY	C3-O11-P1-O14
34	b1	626	SQD	C32-C33-C34-C35
38	b1	625	DGA	CB9-CAB-CBB-CCB
41	C	525	LHG	C11-C12-C13-C14
40	c1	519	DGD	C1A-C2A-C3A-C4A
41	l	101	LHG	C7-C8-C9-C10
41	g	624	LHG	C23-C24-C25-C26
41	n1	624	LHG	C23-C24-C25-C26
35	C	521	LMG	O6-C5-C6-O5
40	C1	519	DGD	O6E-C5E-C6E-O5E
31	b	603	CLA	C3-C5-C6-C7
31	c	507	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	512	CLA	C3-C5-C6-C7
35	a1	413	LMG	C4-C5-C6-O5
34	C1	526	SQD	C10-C11-C12-C13
54	I1	102	4RF	C25-C26-C27-C28
31	B	610	CLA	C13-C15-C16-C17
31	C	505	CLA	C10-C11-C12-C13
31	R	602	CLA	C5-C6-C7-C8
31	b	603	CLA	C15-C16-C17-C18
31	c	502	CLA	C5-C6-C7-C8
31	s	611	CLA	C10-C11-C12-C13
31	B1	614	CLA	C15-C16-C17-C18
31	C1	505	CLA	C10-C11-C12-C13
31	C1	506	CLA	C15-C16-C17-C18
31	b1	604	CLA	C15-C16-C17-C18
31	y1	612	CLA	C8-C10-C11-C12
31	C	508	CLA	CBA-CGA-O2A-C1
34	C	526	SQD	C24-C23-O48-C46
35	c	521	LMG	O6-C5-C6-O5
41	D	409	LHG	O6-C4-C5-C6
41	L	101	LHG	O6-C4-C5-C6
41	G	630	LHG	O6-C4-C5-C6
41	S	624	LHG	O6-C4-C5-C6
41	l	101	LHG	O6-C4-C5-C6
41	n	624	LHG	O6-C4-C5-C6
41	g	624	LHG	O6-C4-C5-C6
41	D1	409	LHG	O6-C4-C5-C6
41	N1	624	LHG	O6-C4-C5-C6
41	G1	624	LHG	O6-C4-C5-C6
41	g1	624	LHG	O6-C4-C5-C6
52	S	626	3PH	O11-C1-C2-C3
57	Y1	627	PTY	O14-C5-C6-C1
35	d	411	LMG	C32-C33-C34-C35
41	G1	624	LHG	C11-C12-C13-C14
52	s	626	3PH	C22-C23-C24-C25
52	S1	626	3PH	C2A-C2B-C2C-C2D
38	B1	625	DGA	CA1-CA2-CA3-CA4
34	b1	626	SQD	C25-C26-C27-C28
41	s	624	LHG	C33-C34-C35-C36
53	a1	414	SPH	C7-C8-C9-C10
54	k1	101	4RF	C03-C04-C05-C06
31	b	612	CLA	C15-C16-C17-C18
31	n1	602	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b	609	CLA	C16-C17-C18-C20
31	b	614	CLA	C16-C17-C18-C19
31	c1	501	CLA	C16-C17-C18-C19
41	S	624	LHG	C28-C29-C30-C31
52	B1	624	3PH	C2C-C2D-C2E-C2F
31	B	612	CLA	O1D-CGD-O2D-CED
34	A	412	SQD	C25-C26-C27-C28
35	W1	201	LMG	C31-C32-C33-C34
41	n1	624	LHG	C13-C14-C15-C16
52	T1	101	3PH	C24-C25-C26-C27
52	T1	101	3PH	C33-C34-C35-C36
52	t1	101	3PH	C2E-C2F-C2G-C2H
31	C	511	CLA	C15-C16-C17-C18
31	y	613	CLA	C8-C10-C11-C12
31	c1	507	CLA	C10-C11-C12-C13
52	S	626	3PH	C3D-C3E-C3F-C3G
51	s1	625	LPX	O1-C3-C4-C5
41	D	410	LHG	O9-C7-O7-C5
41	d1	410	LHG	O9-C7-O7-C5
47	G1	609	CHL	C4-C3-C5-C6
47	y1	609	CHL	C4-C3-C5-C6
34	a	412	SQD	C11-C12-C13-C14
41	C	525	LHG	C10-C11-C12-C13
57	y1	626	PTY	C19-C20-C21-C22
31	C	502	CLA	C13-C15-C16-C17
31	C	513	CLA	C10-C11-C12-C13
31	d	402	CLA	C10-C11-C12-C13
31	G1	602	CLA	C10-C11-C12-C13
31	b1	604	CLA	C8-C10-C11-C12
31	y1	612	CLA	C15-C16-C17-C18
35	A	413	LMG	C18-C19-C20-C21
38	b	623	DGA	CDA-CEA-CFA-CGA
41	d1	409	LHG	C10-C11-C12-C13
41	s1	624	LHG	C34-C35-C36-C37
41	D	409	LHG	C8-C7-O7-C5
57	y1	626	PTY	C11-C8-O7-C6
31	S	610	CLA	O1A-CGA-O2A-C1
31	c	508	CLA	O1A-CGA-O2A-C1
31	C1	508	CLA	O1A-CGA-O2A-C1
40	C1	520	DGD	O1A-C1A-O1G-C1G
40	C	519	DGD	C9B-CAB-CBB-CCB
41	D1	408	LHG	C34-C35-C36-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
52	i	101	3PH	C27-C28-C29-C2A
54	i1	101	4RF	C49-C50-C51-C52
57	Y1	626	PTY	C35-C36-C37-C38
31	C	510	CLA	C2A-CAA-CBA-CGA
31	y	602	CLA	C2A-CAA-CBA-CGA
31	R1	604	CLA	C2A-CAA-CBA-CGA
31	y1	604	CLA	C2A-CAA-CBA-CGA
31	b	608	CLA	C16-C17-C18-C20
31	G1	611	CLA	C16-C17-C18-C20
34	A1	412	SQD	O6-C44-C45-C46
35	C	521	LMG	O1-C7-C8-C9
35	a1	413	LMG	C7-C8-C9-O8
35	h1	102	LMG	C7-C8-C9-O8
40	c1	520	DGD	O1G-C1G-C2G-C3G
41	D	410	LHG	C4-C5-C6-O8
41	L	101	LHG	C4-C5-C6-O8
41	n	624	LHG	C34-C35-C36-C37
41	g	624	LHG	C4-C5-C6-O8
41	y	624	LHG	C4-C5-C6-O8
41	C1	525	LHG	C4-C5-C6-O8
41	D1	409	LHG	C4-C5-C6-O8
41	d1	410	LHG	C4-C5-C6-O8
42	C	527	LMK	O1-C7-C8-C9
42	c	627	LMK	O1-C7-C8-C9
42	C1	527	LMK	O1-C7-C8-C9
42	c1	527	LMK	O1-C7-C8-C9
52	T1	101	3PH	C1-C2-C3-O31
52	b1	624	3PH	C3F-C3G-C3H-C3I
52	s1	626	3PH	C1-C2-C3-O31
55	R1	625	LMT	C3-C4-C5-C6
57	Y1	626	PTY	C36-C37-C38-C39
31	y1	611	CLA	C15-C16-C17-C18
38	C1	524	DGA	CA5-CA6-CA7-CA8
38	c1	524	DGA	CBB-CAB-CB9-CB8
52	i	101	3PH	C34-C35-C36-C37
35	j	101	LMG	C8-C7-O1-C1
35	w1	201	LMG	C8-C7-O1-C1
40	c	519	DGD	C5D-C6D-O5D-C1E
40	C1	519	DGD	C2G-C3G-O3G-C1D
40	c1	519	DGD	C5D-C6D-O5D-C1E
42	c	627	LMK	C8-C9-O8-C28
34	a1	412	SQD	C11-C12-C13-C14

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	B1	625	DGA	CA8-CA9-CAA-CBA
41	D	410	LHG	C25-C26-C27-C28
54	I1	102	4RF	C26-C27-C28-C29
35	a	413	LMG	O6-C5-C6-O5
31	c	505	CLA	O1D-CGD-O2D-CED
31	N	603	CLA	C13-C15-C16-C17
31	b	610	CLA	C15-C16-C17-C18
31	b	617	CLA	C8-C10-C11-C12
31	S1	611	CLA	C13-C15-C16-C17
32	A1	409	PHO	C15-C16-C17-C18
47	Y	606	CHL	C15-C16-C17-C18
38	j1	101	DGA	CB4-CB5-CB6-CB7
41	d	410	LHG	C31-C32-C33-C34
52	S1	626	3PH	C2D-C2E-C2F-C2G
34	B	621	SQD	C23-C24-C25-C26
54	K1	101	4RF	O42-C41-O40-C39
35	D1	411	LMG	C18-C19-C20-C21
57	Y1	626	PTY	C41-C42-C43-C44
31	R	610	CLA	C3-C5-C6-C7
31	R	612	CLA	C3-C5-C6-C7
31	B1	602	CLA	C3-C5-C6-C7
35	j	101	LMG	O6-C1-O1-C7
31	r	610	CLA	C10-C11-C12-C13
31	S1	614	CLA	C5-C6-C7-C8
47	n	601	CHL	C8-C10-C11-C12
44	D	405	PL9	C44-C46-C47-C48
44	D1	405	PL9	C14-C16-C17-C18
38	B	625	DGA	CB3-CB4-CB5-CB6
38	b	623	DGA	CBB-CAB-CB9-CB8
38	B1	625	DGA	CEA-CFA-CGA-CHA
38	b1	625	DGA	CAA-CBA-CCA-CDA
40	C	520	DGD	CCB-CDB-CEB-CFB
35	D	411	LMG	O6-C5-C6-O5
41	N	624	LHG	O1-C1-C2-O2
41	G	630	LHG	O1-C1-C2-O2
41	g	624	LHG	O1-C1-C2-O2
41	d1	408	LHG	O1-C1-C2-O2
38	b	623	DGA	CB7-CB8-CB9-CAB
38	B1	625	DGA	CA5-CA6-CA7-CA8
38	b1	625	DGA	CB3-CB4-CB5-CB6
41	d	409	LHG	C33-C34-C35-C36
53	a1	414	SPH	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N	602	CLA	C13-C15-C16-C17
31	Y	602	CLA	C10-C11-C12-C13
31	r	610	CLA	C5-C6-C7-C8
31	Y1	602	CLA	C15-C16-C17-C18
31	r1	603	CLA	C10-C11-C12-C13
32	a	408	PHO	C8-C10-C11-C12
31	y	602	CLA	O1A-CGA-O2A-C1
35	C1	521	LMG	O6-C5-C6-O5
35	b1	622	LMG	C11-C12-C13-C14
35	w1	201	LMG	C11-C10-O7-C8
38	b1	625	DGA	CA4-CA5-CA6-CA7
41	N	624	LHG	C11-C12-C13-C14
41	c	625	LHG	C11-C12-C13-C14
52	i	101	3PH	C38-C39-C3A-C3B
31	C	509	CLA	C8-C10-C11-C12
31	b	604	CLA	C13-C15-C16-C17
31	c	502	CLA	C13-C15-C16-C17
47	n	601	CHL	C10-C11-C12-C13
35	D1	411	LMG	O6-C5-C6-O5
40	c1	519	DGD	O6E-C5E-C6E-O5E
50	S	622	NEX	C39-C29-C30-C31
31	Y1	603	CLA	C4-C3-C5-C6
31	y1	603	CLA	C4-C3-C5-C6
32	a1	408	PHO	C4-C3-C5-C6
44	d1	405	PL9	C40-C39-C41-C42
34	M1	101	SQD	C28-C29-C30-C31
41	C	525	LHG	C34-C35-C36-C37
41	d	408	LHG	C30-C31-C32-C33
41	Y1	624	LHG	C35-C36-C37-C38
40	C1	519	DGD	O1A-C1A-O1G-C1G
52	s1	626	3PH	O32-C31-O31-C3
31	Y1	603	CLA	C2-C3-C5-C6
31	c1	510	CLA	C2-C3-C5-C6
31	y1	603	CLA	C2-C3-C5-C6
32	a1	408	PHO	C2-C3-C5-C6
40	C1	520	DGD	C1B-C2B-C3B-C4B
31	n	610	CLA	C16-C17-C18-C20
31	c1	513	CLA	C16-C17-C18-C20
31	D	402	CLA	CBA-CGA-O2A-C1
31	N	602	CLA	CBA-CGA-O2A-C1
31	b1	617	CLA	CBA-CGA-O2A-C1
41	c	625	LHG	C24-C23-O8-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
54	k1	101	4RF	C15-C16-O18-C19
35	H1	102	LMG	O6-C5-C6-O5
35	h1	102	LMG	O6-C5-C6-O5
40	B1	623	DGD	O6E-C5E-C6E-O5E
34	a1	412	SQD	C35-C36-C37-C38
38	C	524	DGA	CB2-CB3-CB4-CB5
41	C	525	LHG	C35-C36-C37-C38
52	S	626	3PH	C23-C24-C25-C26
31	n	604	CLA	CBD-CGD-O2D-CED
31	C	513	CLA	C15-C16-C17-C18
31	R	603	CLA	C8-C10-C11-C12
31	B1	605	CLA	C15-C16-C17-C18
31	C1	510	CLA	C5-C6-C7-C8
41	g	624	LHG	O8-C23-C24-C25
34	m1	101	SQD	C11-C10-C9-C8
35	C1	523	LMG	C13-C14-C15-C16
40	C1	519	DGD	C4B-C5B-C6B-C7B
41	N	624	LHG	C30-C31-C32-C33
41	S	624	LHG	C31-C32-C33-C34
41	G1	624	LHG	C33-C34-C35-C36
52	S	626	3PH	C3F-C3G-C3H-C3I
54	K1	101	4RF	C05-C06-C07-C08
34	M1	101	SQD	C46-C45-O47-C7
35	B	622	LMG	C9-C8-O7-C10
35	W1	201	LMG	C7-C8-O7-C10
38	b	623	DGA	CG1-CG2-OG2-CB1
40	c	523	DGD	C1G-C2G-O2G-C1B
52	T1	101	3PH	C3-C2-O21-C21
31	D	402	CLA	C2A-CAA-CBA-CGA
31	n	604	CLA	C5-C6-C7-C8
31	b1	603	CLA	C13-C15-C16-C17
31	b1	611	CLA	C10-C11-C12-C13
31	g1	602	CLA	C8-C10-C11-C12
31	A	407	CLA	C2-C1-O2A-CGA
31	b	616	CLA	C2-C1-O2A-CGA
31	c	503	CLA	C2-C1-O2A-CGA
31	n	614	CLA	C2-C1-O2A-CGA
31	r	604	CLA	C2-C1-O2A-CGA
31	r	608	CLA	C2-C1-O2A-CGA
31	s	603	CLA	C2-C1-O2A-CGA
31	y	608	CLA	C2-C1-O2A-CGA
31	C1	504	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	S1	611	CLA	C2-C1-O2A-CGA
31	Y1	602	CLA	C2-C1-O2A-CGA
31	Y1	611	CLA	C2-C1-O2A-CGA
31	b1	605	CLA	C2-C1-O2A-CGA
31	n1	613	CLA	C2-C1-O2A-CGA
31	n1	614	CLA	C2-C1-O2A-CGA
31	r1	604	CLA	C2-C1-O2A-CGA
31	s1	610	CLA	C2-C1-O2A-CGA
31	s1	611	CLA	C2-C1-O2A-CGA
31	y1	602	CLA	C2-C1-O2A-CGA
34	B	621	SQD	C31-C32-C33-C34
38	j1	101	DGA	CA7-CA8-CA9-CAA
41	C1	525	LHG	C35-C36-C37-C38
41	D1	409	LHG	C35-C36-C37-C38
41	D1	410	LHG	C11-C10-C9-C8
52	s1	626	3PH	C29-C2A-C2B-C2C
35	c1	521	LMG	O6-C5-C6-O5
31	r1	609	CLA	C3-C5-C6-C7
41	N	624	LHG	C11-C10-C9-C8
41	N1	624	LHG	C9-C10-C11-C12
41	g1	624	LHG	C11-C12-C13-C14
53	A1	414	SPH	C10-C11-C12-C13
31	b	607	CLA	C13-C15-C16-C17
31	C1	504	CLA	C15-C16-C17-C18
31	D1	403	CLA	C15-C16-C17-C18
41	C	525	LHG	C2-C3-O3-P
52	T1	101	3PH	C1-O11-P-O12
52	S1	626	3PH	C1-O11-P-O12
38	c	524	DGA	CB7-CB8-CB9-CAB
38	c1	524	DGA	CDB-CEB-CFB-CGB
41	l	101	LHG	C35-C36-C37-C38
52	t1	101	3PH	C25-C26-C27-C28
53	a1	414	SPH	C10-C11-C12-C13
31	B	604	CLA	CBA-CGA-O2A-C1
31	S	611	CLA	CBA-CGA-O2A-C1
31	R1	612	CLA	CBA-CGA-O2A-C1
31	c1	501	CLA	CBA-CGA-O2A-C1
32	a	408	PHO	CBA-CGA-O2A-C1
54	I1	102	4RF	C43-C41-O40-C39
41	n	624	LHG	O6-C4-C5-O7
52	s	626	3PH	O11-C1-C2-O21
31	S1	604	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	Y1	611	CLA	C16-C17-C18-C19
54	I1	102	4RF	C41-C43-C44-C45
38	C	524	DGA	CB7-CB8-CB9-CAB
41	s	624	LHG	C27-C28-C29-C30
41	y	624	LHG	C11-C12-C13-C14
52	i	101	3PH	C3B-C3C-C3D-C3E
52	t1	101	3PH	C3A-C3B-C3C-C3D
52	s1	626	3PH	C34-C35-C36-C37
47	r	606	CHL	C2A-CAA-CBA-CGA
31	n	610	CLA	C13-C15-C16-C17
47	S	608	CHL	C5-C6-C7-C8
40	c	523	DGD	CAB-CBB-CCB-CDB
31	C1	502	CLA	O1A-CGA-O2A-C1
34	M1	101	SQD	C12-C13-C14-C15
41	Y	624	LHG	C25-C26-C27-C28
41	N1	624	LHG	C11-C12-C13-C14
41	d1	410	LHG	C28-C29-C30-C31
41	n	624	LHG	C23-C24-C25-C26
41	d1	410	LHG	C7-C8-C9-C10
31	c	513	CLA	C8-C10-C11-C12
31	B1	614	CLA	C13-C15-C16-C17
31	C1	506	CLA	C10-C11-C12-C13
31	C1	512	CLA	C13-C15-C16-C17
31	s1	614	CLA	C5-C6-C7-C8
40	b1	623	DGD	C2D-C1D-O3G-C3G
35	D1	411	LMG	C19-C20-C21-C22
41	L	101	LHG	C25-C26-C27-C28
41	N	624	LHG	C35-C36-C37-C38
41	S	624	LHG	C34-C35-C36-C37
55	r1	625	LMT	C4'-C5'-C6'-O6'
35	h1	102	LMG	O7-C8-C9-O8
38	C	524	DGA	OG1-CG1-CG2-OG2
38	j1	101	DGA	OG1-CG1-CG2-OG2
41	y	624	LHG	O7-C5-C6-O8
31	S	602	CLA	O1D-CGD-O2D-CED
34	C1	526	SQD	C26-C27-C28-C29
41	Y	624	LHG	C31-C32-C33-C34
41	l	101	LHG	C34-C35-C36-C37
52	B1	624	3PH	O22-C21-O21-C2
31	S	610	CLA	C8-C10-C11-C12
31	B1	611	CLA	C8-C10-C11-C12
31	S1	609	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C	508	CLA	O1A-CGA-O2A-C1
31	c	509	CLA	O1A-CGA-O2A-C1
34	C	526	SQD	O10-C23-O48-C46
31	B	616	CLA	C16-C17-C18-C19
31	s1	604	CLA	C6-C7-C8-C10
32	a1	409	PHO	CHA-CBD-CGD-O1D
32	a1	409	PHO	CHA-CBD-CGD-O2D
34	a1	412	SQD	C13-C14-C15-C16
35	h1	102	LMG	C37-C38-C39-C40
38	b1	625	DGA	CFB-CGB-CHB-CIB
40	C1	520	DGD	CCB-CDB-CEB-CFB
54	k1	101	4RF	C35-C36-C37-C38
35	D	411	LMG	C28-C29-C30-C31
31	G	602	CLA	C4-C3-C5-C6
31	G1	613	CLA	C4-C3-C5-C6
31	Y1	604	CLA	C4-C3-C5-C6
31	c1	510	CLA	C4-C3-C5-C6
47	G1	607	CHL	C4-C3-C5-C6
38	b	623	DGA	CAA-CBA-CCA-CDA
51	S1	625	LPX	C14-C15-C16-C17
52	s	626	3PH	C36-C37-C38-C39
31	s	610	CLA	C15-C16-C17-C18
31	B	602	CLA	C11-C10-C8-C7
31	B	603	CLA	C6-C7-C8-C10
31	B	608	CLA	C12-C13-C15-C16
31	B	614	CLA	C11-C12-C13-C15
31	C	501	CLA	C11-C12-C13-C15
31	C	505	CLA	C12-C13-C15-C16
31	C	506	CLA	C11-C10-C8-C7
31	C	507	CLA	C11-C12-C13-C15
31	C	508	CLA	C11-C10-C8-C7
31	C	513	CLA	C6-C7-C8-C10
31	D	402	CLA	C11-C10-C8-C7
31	D	402	CLA	C11-C12-C13-C15
31	D	403	CLA	C11-C12-C13-C15
31	N	613	CLA	C11-C12-C13-C15
31	G	603	CLA	C11-C12-C13-C15
31	G	613	CLA	C6-C7-C8-C10
31	S	610	CLA	C11-C12-C13-C15
31	S	611	CLA	C6-C7-C8-C10
31	S	611	CLA	C11-C12-C13-C15
31	a	405	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b	602	CLA	C11-C10-C8-C7
31	b	603	CLA	C6-C7-C8-C10
31	b	605	CLA	C11-C10-C8-C7
31	b	607	CLA	C11-C12-C13-C15
31	b	613	CLA	C11-C10-C8-C7
31	b	616	CLA	C11-C12-C13-C15
31	c	502	CLA	C6-C7-C8-C10
31	c	506	CLA	C11-C10-C8-C7
31	c	507	CLA	C11-C10-C8-C7
31	c	510	CLA	C6-C7-C8-C10
31	c	511	CLA	C11-C12-C13-C15
31	c	512	CLA	C6-C7-C8-C10
31	c	513	CLA	C6-C7-C8-C10
31	c	513	CLA	C11-C12-C13-C15
31	n	603	CLA	C6-C7-C8-C10
31	n	603	CLA	C11-C12-C13-C15
31	n	610	CLA	C6-C7-C8-C10
31	n	613	CLA	C11-C12-C13-C15
31	g	602	CLA	C6-C7-C8-C10
31	g	603	CLA	C12-C13-C15-C16
31	g	613	CLA	C6-C7-C8-C10
31	g	613	CLA	C11-C10-C8-C7
31	r	603	CLA	C11-C10-C8-C7
31	r	609	CLA	C6-C7-C8-C10
31	s	609	CLA	C11-C10-C8-C7
31	s	610	CLA	C11-C10-C8-C7
31	s	611	CLA	C2-C3-C5-C6
31	y	602	CLA	C6-C7-C8-C10
31	B1	604	CLA	C6-C7-C8-C10
31	B1	604	CLA	C11-C10-C8-C7
31	B1	607	CLA	C11-C10-C8-C7
31	C1	502	CLA	C11-C12-C13-C15
31	C1	505	CLA	C11-C12-C13-C15
31	C1	506	CLA	C12-C13-C15-C16
31	C1	507	CLA	C12-C13-C15-C16
31	C1	509	CLA	C12-C13-C15-C16
31	C1	510	CLA	C12-C13-C15-C16
31	C1	513	CLA	C11-C12-C13-C15
31	D1	402	CLA	C11-C12-C13-C15
31	D1	403	CLA	C11-C12-C13-C15
31	N1	602	CLA	C6-C7-C8-C10
31	N1	610	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N1	610	CLA	C12-C13-C15-C16
31	G1	602	CLA	C6-C7-C8-C10
31	G1	603	CLA	C6-C7-C8-C10
31	G1	610	CLA	C11-C10-C8-C7
31	R1	610	CLA	C11-C10-C8-C7
31	S1	609	CLA	C6-C7-C8-C10
31	S1	611	CLA	C11-C12-C13-C15
31	Y1	603	CLA	C12-C13-C15-C16
31	Y1	604	CLA	C2-C3-C5-C6
31	Y1	610	CLA	C11-C12-C13-C15
31	Y1	613	CLA	C11-C12-C13-C15
31	Y1	613	CLA	C12-C13-C15-C16
31	a1	405	CLA	C11-C12-C13-C15
31	a1	406	CLA	C12-C13-C15-C16
31	b1	603	CLA	C6-C7-C8-C10
31	b1	604	CLA	C11-C12-C13-C15
31	b1	607	CLA	C11-C12-C13-C15
31	c1	507	CLA	C12-C13-C15-C16
31	c1	509	CLA	C6-C7-C8-C10
31	c1	510	CLA	C12-C13-C15-C16
31	d1	402	CLA	C11-C10-C8-C7
31	n1	603	CLA	C11-C10-C8-C7
31	n1	610	CLA	C11-C12-C13-C15
31	n1	610	CLA	C12-C13-C15-C16
31	g1	603	CLA	C6-C7-C8-C10
31	g1	603	CLA	C12-C13-C15-C16
31	g1	610	CLA	C11-C10-C8-C7
31	g1	611	CLA	C6-C7-C8-C10
31	s1	609	CLA	C11-C10-C8-C7
31	y1	602	CLA	C6-C7-C8-C10
31	y1	612	CLA	C11-C10-C8-C7
31	y1	613	CLA	C11-C12-C13-C15
32	A	409	PHO	C6-C7-C8-C10
47	N	606	CHL	C11-C10-C8-C7
47	Y	601	CHL	C11-C10-C8-C7
47	Y	607	CHL	C2-C3-C5-C6
47	Y	607	CHL	C11-C10-C8-C7
47	n	605	CHL	C11-C12-C13-C15
47	n	606	CHL	C11-C12-C13-C15
47	N1	607	CHL	C11-C12-C13-C15
47	G1	601	CHL	C12-C13-C15-C16
47	G1	607	CHL	C2-C3-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	S1	608	CHL	C11-C10-C8-C7
47	Y1	606	CHL	C11-C12-C13-C15
47	Y1	607	CHL	C12-C13-C15-C16
47	Y1	609	CHL	C11-C12-C13-C15
47	Y1	609	CHL	C12-C13-C15-C16
47	n1	605	CHL	C12-C13-C15-C16
47	n1	607	CHL	C11-C12-C13-C15
47	y1	609	CHL	C2-C3-C5-C6
47	y1	609	CHL	C12-C13-C15-C16
35	c1	521	LMG	O7-C10-C11-C12
31	S	611	CLA	O1A-CGA-O2A-C1
34	C	526	SQD	C9-C10-C11-C12
40	C	523	DGD	CDA-CEA-CFA-CGA
41	C	525	LHG	C30-C31-C32-C33
41	D	408	LHG	C11-C12-C13-C14
52	s	626	3PH	C3D-C3E-C3F-C3G
31	B	603	CLA	C6-C7-C8-C9
31	B	603	CLA	C11-C10-C8-C9
31	B	603	CLA	C14-C13-C15-C16
31	B	607	CLA	C6-C7-C8-C9
31	B	608	CLA	C14-C13-C15-C16
31	C	501	CLA	C11-C10-C8-C9
31	C	507	CLA	C14-C13-C15-C16
31	C	512	CLA	C11-C10-C8-C9
31	C	513	CLA	C6-C7-C8-C9
31	D	402	CLA	C11-C10-C8-C9
31	D	402	CLA	C11-C12-C13-C14
31	D	403	CLA	C11-C12-C13-C14
31	N	613	CLA	C11-C12-C13-C14
31	G	602	CLA	C6-C7-C8-C9
31	G	603	CLA	C11-C12-C13-C14
31	S	611	CLA	C6-C7-C8-C9
31	S	611	CLA	C11-C12-C13-C14
31	Y	611	CLA	C11-C10-C8-C9
31	a	405	CLA	C11-C12-C13-C14
31	b	602	CLA	C6-C7-C8-C9
31	b	602	CLA	C11-C10-C8-C9
31	b	603	CLA	C6-C7-C8-C9
31	b	604	CLA	C11-C12-C13-C14
31	c	507	CLA	C11-C12-C13-C14
31	c	507	CLA	C14-C13-C15-C16
31	c	510	CLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	511	CLA	C11-C12-C13-C14
31	c	512	CLA	C6-C7-C8-C9
31	c	512	CLA	C11-C12-C13-C14
31	c	512	CLA	C14-C13-C15-C16
31	c	513	CLA	C6-C7-C8-C9
31	n	604	CLA	C11-C10-C8-C9
31	g	602	CLA	C6-C7-C8-C9
31	g	603	CLA	C11-C12-C13-C14
31	g	603	CLA	C14-C13-C15-C16
31	g	613	CLA	C6-C7-C8-C9
31	g	613	CLA	C11-C10-C8-C9
31	g	613	CLA	C14-C13-C15-C16
31	y	610	CLA	C6-C7-C8-C9
31	A1	406	CLA	C14-C13-C15-C16
31	B1	605	CLA	C11-C10-C8-C9
31	B1	607	CLA	C11-C10-C8-C9
31	C1	502	CLA	C11-C12-C13-C14
31	C1	504	CLA	C11-C10-C8-C9
31	C1	505	CLA	C14-C13-C15-C16
31	C1	509	CLA	C14-C13-C15-C16
31	C1	510	CLA	C6-C7-C8-C9
31	C1	510	CLA	C14-C13-C15-C16
31	C1	513	CLA	C11-C12-C13-C14
31	D1	402	CLA	C11-C12-C13-C14
31	D1	403	CLA	C11-C12-C13-C14
31	N1	602	CLA	C6-C7-C8-C9
31	G1	602	CLA	C6-C7-C8-C9
31	G1	610	CLA	C11-C10-C8-C9
31	G1	610	CLA	C11-C12-C13-C14
31	G1	611	CLA	C6-C7-C8-C9
31	G1	613	CLA	C14-C13-C15-C16
31	S1	610	CLA	C11-C10-C8-C9
31	Y1	602	CLA	C6-C7-C8-C9
31	Y1	602	CLA	C11-C12-C13-C14
31	Y1	613	CLA	C14-C13-C15-C16
31	a1	405	CLA	C11-C12-C13-C14
31	b1	604	CLA	C6-C7-C8-C9
31	c1	501	CLA	C14-C13-C15-C16
31	c1	503	CLA	C14-C13-C15-C16
31	c1	505	CLA	C14-C13-C15-C16
31	c1	509	CLA	C14-C13-C15-C16
31	c1	512	CLA	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	d1	402	CLA	C11-C10-C8-C9
31	n1	603	CLA	C11-C10-C8-C9
31	n1	603	CLA	C14-C13-C15-C16
31	n1	610	CLA	C11-C12-C13-C14
31	n1	610	CLA	C14-C13-C15-C16
31	g1	603	CLA	C6-C7-C8-C9
31	r1	609	CLA	C11-C10-C8-C9
31	y1	602	CLA	C6-C7-C8-C9
31	y1	603	CLA	C6-C7-C8-C9
31	y1	610	CLA	C11-C12-C13-C14
31	y1	613	CLA	C11-C10-C8-C9
47	N	605	CHL	C11-C10-C8-C9
47	G	609	CHL	C11-C12-C13-C14
47	G	609	CHL	C14-C13-C15-C16
47	Y	601	CHL	C11-C12-C13-C14
47	y	606	CHL	C11-C10-C8-C9
47	y	607	CHL	C11-C12-C13-C14
47	y	609	CHL	C14-C13-C15-C16
47	N1	605	CHL	C11-C10-C8-C9
47	N1	606	CHL	C11-C10-C8-C9
47	G1	609	CHL	C14-C13-C15-C16
47	S1	608	CHL	C11-C10-C8-C9
47	Y1	606	CHL	C6-C7-C8-C9
47	Y1	606	CHL	C11-C12-C13-C14
47	n1	607	CHL	C11-C12-C13-C14
33	a1	411	BCR	C19-C20-C21-C22
48	s1	621	LUT	C29-C30-C31-C32
49	g	622	XAT	C14-C15-C35-C34
34	B	621	SQD	C7-C8-C9-C10
57	Y1	626	PTY	C8-C11-C12-C13
35	a	413	LMG	C32-C33-C34-C35
38	C	524	DGA	CBB-CAB-CB9-CB8
38	B1	625	DGA	CB7-CB8-CB9-CAB
40	c1	519	DGD	C4B-C5B-C6B-C7B
41	d	409	LHG	C13-C14-C15-C16
41	d	409	LHG	C17-C18-C19-C20
41	G1	624	LHG	C31-C32-C33-C34
52	t1	101	3PH	C2D-C2E-C2F-C2G
52	s1	626	3PH	C2B-C2C-C2D-C2E
31	Y	610	CLA	CBA-CGA-O2A-C1
35	C	521	LMG	C29-C28-O8-C9
54	k1	101	4RF	C43-C41-O40-C39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	512	CLA	C15-C16-C17-C18
31	Y	602	CLA	C2A-CAA-CBA-CGA
31	S1	617	CLA	C2A-CAA-CBA-CGA
34	A	412	SQD	C30-C31-C32-C33
41	G1	624	LHG	C16-C17-C18-C19
41	Y1	624	LHG	C33-C34-C35-C36
44	D1	405	PL9	C47-C48-C49-C50
31	c1	501	CLA	O1A-CGA-O2A-C1
37	b	620	C7Z	C7-C8-C9-C19
48	G1	620	LUT	C27-C28-C29-C39
31	B1	603	CLA	C13-C15-C16-C17
31	B	602	CLA	C16-C17-C18-C19
31	G	603	CLA	C16-C17-C18-C19
31	Y	613	CLA	C16-C17-C18-C19
31	B1	607	CLA	C16-C17-C18-C19
31	D1	403	CLA	C16-C17-C18-C20
31	b1	605	CLA	C16-C17-C18-C19
33	C	514	BCR	C11-C12-C13-C14
33	a1	411	BCR	C7-C8-C9-C10
37	b	620	C7Z	C7-C8-C9-C10
49	y	622	XAT	C11-C12-C13-C14
49	n1	622	XAT	C27-C28-C29-C30
49	y1	622	XAT	C27-C28-C29-C30
38	C1	524	DGA	CBA-CCA-CDA-CEA
38	c1	524	DGA	CBB-CCB-CDB-CEB
40	c	518	DGD	C6B-C7B-C8B-C9B
41	D1	410	LHG	C31-C32-C33-C34
54	K1	101	4RF	C24-C25-C26-C27
41	s1	624	LHG	C1-C2-C3-O3
31	b1	612	CLA	C15-C16-C17-C18
31	s1	603	CLA	C10-C11-C12-C13
38	B	625	DGA	CFA-CGA-CHA-CIA
38	c	524	DGA	CB2-CB3-CB4-CB5
40	C	520	DGD	CAB-CBB-CCB-CDB
42	C	527	LMK	C29-C30-C31-C32
31	b1	617	CLA	O1A-CGA-O2A-C1
31	G	610	CLA	CBA-CGA-O2A-C1
31	y	610	CLA	CBA-CGA-O2A-C1
31	s1	609	CLA	CBA-CGA-O2A-C1
38	j1	101	DGA	CA2-CA1-OG1-CG1
41	g1	624	LHG	C16-C17-C18-C19
52	B1	624	3PH	C38-C39-C3A-C3B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
52	T1	101	3PH	C34-C35-C36-C37
31	C	512	CLA	C13-C15-C16-C17
31	c	501	CLA	C15-C16-C17-C18
31	n	602	CLA	C13-C15-C16-C17
31	B1	612	CLA	C13-C15-C16-C17
31	Y1	613	CLA	C15-C16-C17-C18
31	Y1	614	CLA	C8-C10-C11-C12
31	b1	605	CLA	O1D-CGD-O2D-CED
40	c	520	DGD	C4E-C5E-C6E-O5E
38	C	524	DGA	CA8-CA9-CAA-CBA
41	s	624	LHG	C28-C29-C30-C31
41	d1	410	LHG	C30-C31-C32-C33
41	g1	624	LHG	C11-C10-C9-C8
54	I1	102	4RF	C49-C50-C51-C52
54	k1	101	4RF	C44-C45-C46-C47
35	w1	201	LMG	O7-C10-C11-C12
40	c	519	DGD	O6D-C5D-C6D-O5D
40	B1	623	DGD	O6D-C5D-C6D-O5D
40	c1	518	DGD	C3B-C4B-C5B-C6B
41	L	101	LHG	C28-C29-C30-C31
41	Y1	624	LHG	C30-C31-C32-C33
41	y1	624	LHG	C26-C27-C28-C29
31	b	609	CLA	C16-C17-C18-C19
40	C1	518	DGD	C2G-C1G-O1G-C1A
34	c1	526	SQD	O5-C1-O6-C44
31	C	510	CLA	C13-C15-C16-C17
31	N1	613	CLA	C13-C15-C16-C17
31	c1	505	CLA	C13-C15-C16-C17
31	c1	507	CLA	C15-C16-C17-C18
31	n1	604	CLA	C15-C16-C17-C18
31	r1	602	CLA	C10-C11-C12-C13
31	y1	613	CLA	C5-C6-C7-C8
41	C	525	LHG	O6-C4-C5-C6
41	D	408	LHG	O6-C4-C5-C6
41	c	625	LHG	O6-C4-C5-C6
41	d	408	LHG	O6-C4-C5-C6
41	d	410	LHG	O6-C4-C5-C6
41	C1	525	LHG	O6-C4-C5-C6
41	L1	101	LHG	O6-C4-C5-C6
41	c1	525	LHG	O6-C4-C5-C6
41	d1	408	LHG	O6-C4-C5-C6
41	d1	409	LHG	O6-C4-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
52	i	101	3PH	O11-C1-C2-C3
52	B1	624	3PH	O11-C1-C2-C3
38	C	524	DGA	CB3-CB4-CB5-CB6
41	n	624	LHG	C11-C12-C13-C14
52	i	101	3PH	C3E-C3F-C3G-C3H
35	c	521	LMG	C28-C29-C30-C31
40	C1	519	DGD	C1A-C2A-C3A-C4A
49	N	622	XAT	C26-C27-C28-C29
34	C1	526	SQD	C33-C34-C35-C36
38	C1	524	DGA	CB4-CB5-CB6-CB7
41	D	409	LHG	C30-C31-C32-C33
41	n	624	LHG	C25-C26-C27-C28
41	D1	409	LHG	C31-C32-C33-C34
31	b	608	CLA	C13-C15-C16-C17
31	c	512	CLA	C13-C15-C16-C17
31	c1	506	CLA	C8-C10-C11-C12
35	C	521	LMG	C11-C12-C13-C14
42	C1	527	LMK	C11-C12-C13-C14
54	K1	101	4RF	C52-C53-C54-C55
31	R	602	CLA	C4-C3-C5-C6
31	C1	510	CLA	C4-C3-C5-C6
31	c1	508	CLA	C4-C3-C5-C6
31	n	603	CLA	C2-C3-C5-C6
31	G1	613	CLA	C2-C3-C5-C6
35	H	102	LMG	C28-C29-C30-C31
40	c	519	DGD	C6B-C7B-C8B-C9B
41	c1	525	LHG	C25-C26-C27-C28
41	y1	624	LHG	C30-C31-C32-C33
54	k1	101	4RF	C12-C13-C14-C15
31	B1	617	CLA	C5-C6-C7-C8
31	B	604	CLA	O1A-CGA-O2A-C1
31	D	402	CLA	O1A-CGA-O2A-C1
35	w1	201	LMG	C36-C37-C38-C39
41	S	624	LHG	C11-C10-C9-C8
41	c	625	LHG	C33-C34-C35-C36
41	d	408	LHG	C11-C10-C9-C8
31	b	608	CLA	C16-C17-C18-C19
31	b	614	CLA	C16-C17-C18-C20
31	d	402	CLA	C16-C17-C18-C20
41	D1	408	LHG	C24-C25-C26-C27
41	S1	624	LHG	C31-C32-C33-C34
41	d1	410	LHG	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
52	S	626	3PH	C27-C28-C29-C2A
52	T1	101	3PH	C3F-C3G-C3H-C3I
31	C1	507	CLA	C15-C16-C17-C18
47	G	601	CHL	C10-C11-C12-C13
31	s	604	CLA	CBA-CGA-O2A-C1
31	A1	405	CLA	CBA-CGA-O2A-C1
31	B1	612	CLA	CBA-CGA-O2A-C1
31	c1	502	CLA	CBA-CGA-O2A-C1
31	r1	610	CLA	CBA-CGA-O2A-C1
32	A1	408	PHO	CBA-CGA-O2A-C1
38	C1	524	DGA	CA2-CA1-OG1-CG1
41	d1	408	LHG	C24-C23-O8-C6
31	b1	605	CLA	CAA-CBA-CGA-O2A
34	m1	101	SQD	O47-C7-C8-C9
41	n	624	LHG	O8-C23-C24-C25
34	b	621	SQD	C7-C8-C9-C10
38	b1	625	DGA	CBB-CAB-CB9-CB8
41	D	409	LHG	C25-C26-C27-C28
41	S	624	LHG	C14-C15-C16-C17
42	c	627	LMK	C29-C30-C31-C32
41	d	410	LHG	C2-C3-O3-P
31	N	604	CLA	C3A-C2A-CAA-CBA
31	N	613	CLA	C3A-C2A-CAA-CBA
31	R	604	CLA	C3A-C2A-CAA-CBA
31	c	506	CLA	C3A-C2A-CAA-CBA
31	n	613	CLA	C3A-C2A-CAA-CBA
31	B1	602	CLA	C3A-C2A-CAA-CBA
31	B1	610	CLA	C3A-C2A-CAA-CBA
31	N1	614	CLA	C3A-C2A-CAA-CBA
31	S1	605	CLA	C3A-C2A-CAA-CBA
31	c1	505	CLA	C3A-C2A-CAA-CBA
32	a	409	PHO	C3A-C2A-CAA-CBA
47	g	606	CHL	C3A-C2A-CAA-CBA
47	n1	601	CHL	C3A-C2A-CAA-CBA
38	C	524	DGA	CB9-CAB-CBB-CCB
40	C1	519	DGD	C2A-C3A-C4A-C5A
33	C	514	BCR	C13-C14-C15-C16
33	A1	411	BCR	C19-C20-C21-C22
33	B1	618	BCR	C13-C14-C15-C16
33	C1	514	BCR	C15-C16-C17-C18
48	N	621	LUT	C29-C30-C31-C32
48	N1	620	LUT	C9-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
48	Y1	621	LUT	C29-C30-C31-C32
49	r	622	XAT	C9-C10-C11-C12
50	R	622	NEX	C33-C34-C35-C15
34	a1	412	SQD	C24-C25-C26-C27
34	b1	626	SQD	C12-C13-C14-C15
40	c1	518	DGD	C2A-C3A-C4A-C5A
41	c	625	LHG	C9-C10-C11-C12
57	Y1	626	PTY	C11-C12-C13-C14
31	B1	617	CLA	C3-C5-C6-C7
31	R1	608	CLA	C3-C5-C6-C7
31	N	613	CLA	C15-C16-C17-C18
31	S	602	CLA	C5-C6-C7-C8
31	y	602	CLA	C13-C15-C16-C17
32	a	408	PHO	C15-C16-C17-C18
35	D1	411	LMG	C32-C33-C34-C35
41	y	624	LHG	C32-C33-C34-C35
31	A	406	CLA	O1D-CGD-O2D-CED
31	S	614	CLA	CBA-CGA-O2A-C1
31	G1	610	CLA	CBA-CGA-O2A-C1
31	n1	610	CLA	CBA-CGA-O2A-C1
34	b1	621	SQD	C24-C23-O48-C46
34	B	621	SQD	C30-C31-C32-C33
41	c1	525	LHG	C35-C36-C37-C38
31	c	503	CLA	C8-C10-C11-C12
34	B1	626	SQD	O6-C44-C45-C46
34	B1	626	SQD	C44-C45-C46-O48
34	b1	626	SQD	O6-C44-C45-C46
34	m1	101	SQD	C44-C45-C46-O48
35	A	413	LMG	C7-C8-C9-O8
35	H	102	LMG	C7-C8-C9-O8
35	a	413	LMG	O1-C7-C8-C9
35	b	622	LMG	C7-C8-C9-O8
35	c	521	LMG	O1-C7-C8-C9
35	h	102	LMG	C7-C8-C9-O8
35	a1	413	LMG	O1-C7-C8-C9
35	w1	201	LMG	O1-C7-C8-C9
38	C	524	DGA	OG1-CG1-CG2-CG3
40	c	523	DGD	O1G-C1G-C2G-C3G
40	b1	623	DGD	O1G-C1G-C2G-C3G
41	G	630	LHG	C4-C5-C6-O8
41	d	410	LHG	C4-C5-C6-O8
41	l	101	LHG	C4-C5-C6-O8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	D1	410	LHG	C4-C5-C6-O8
41	L1	101	LHG	C4-C5-C6-O8
41	G1	624	LHG	C4-C5-C6-O8
41	d1	409	LHG	C4-C5-C6-O8
41	s1	624	LHG	C4-C5-C6-O8
48	N	621	LUT	C21-C26-C27-C28
54	K1	101	4RF	C19-C20-C39-O40
54	i1	101	4RF	C19-C20-C39-O40
54	k1	101	4RF	O18-C19-C20-C39
57	y1	627	PTY	O4-C1-C6-C5
34	A1	412	SQD	C9-C10-C11-C12
41	n1	624	LHG	C35-C36-C37-C38
52	B1	624	3PH	C2F-C2G-C2H-C2I
31	N	602	CLA	O1A-CGA-O2A-C1
41	n	624	LHG	C30-C31-C32-C33
41	G1	624	LHG	C35-C36-C37-C38
34	c1	526	SQD	C32-C33-C34-C35
41	d	408	LHG	C34-C35-C36-C37
53	Y	625	SPH	C10-C11-C12-C13
34	C1	526	SQD	C19-C20-C21-C22
38	J1	101	DGA	CB2-CB3-CB4-CB5
41	n1	624	LHG	C14-C15-C16-C17
52	B1	624	3PH	C2B-C2C-C2D-C2E
54	k1	101	4RF	O17-C16-O18-C19
31	c1	508	CLA	C10-C11-C12-C13
31	c	510	CLA	C4-C3-C5-C6
31	C1	512	CLA	C4-C3-C5-C6
31	G1	611	CLA	C16-C17-C18-C19
31	s	602	CLA	C2-C3-C5-C6
41	g1	624	LHG	C35-C36-C37-C38
40	c	520	DGD	O6E-C5E-C6E-O5E
38	C1	524	DGA	CAA-CBA-CCA-CDA
40	c	520	DGD	C2A-C3A-C4A-C5A
41	d	409	LHG	C34-C35-C36-C37
53	y	625	SPH	C10-C11-C12-C13
57	y1	626	PTY	C23-C24-C25-C26
31	D1	403	CLA	C10-C11-C12-C13
31	G1	602	CLA	C5-C6-C7-C8
31	y1	614	CLA	C13-C15-C16-C17
41	L1	101	LHG	C3-O3-P-O6
41	s1	624	LHG	C3-O3-P-O6
42	C	527	LMK	C9-C8-O7-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
42	c	627	LMK	C9-C8-O7-C10
42	C1	527	LMK	C9-C8-O7-C10
57	Y1	627	PTY	C5-O14-P1-O11
41	S1	624	LHG	C23-C24-C25-C26
31	R1	612	CLA	O1A-CGA-O2A-C1
35	C	521	LMG	O10-C28-O8-C9
31	c	513	CLA	C3-C5-C6-C7
31	r	610	CLA	C3-C5-C6-C7
31	a1	410	CLA	C3-C5-C6-C7
35	d	411	LMG	C4-C5-C6-O5
41	D1	409	LHG	O1-C1-C2-O2
31	y	612	CLA	C13-C15-C16-C17
31	b1	615	CLA	C15-C16-C17-C18
35	a1	413	LMG	C30-C31-C32-C33
41	C	525	LHG	C12-C13-C14-C15
41	g	624	LHG	C9-C10-C11-C12
52	b1	624	3PH	C34-C35-C36-C37
41	D	408	LHG	O6-C4-C5-O7
41	D	409	LHG	O6-C4-C5-O7
41	L	101	LHG	O6-C4-C5-O7
41	c	625	LHG	O6-C4-C5-O7
41	d	409	LHG	O6-C4-C5-O7
41	s	624	LHG	O6-C4-C5-O7
41	d1	409	LHG	O6-C4-C5-O7
41	n1	624	LHG	O6-C4-C5-O7
41	g1	624	LHG	O6-C4-C5-O7
52	S	626	3PH	O11-C1-C2-O21
52	t1	101	3PH	O11-C1-C2-O21
57	y1	627	PTY	O14-C5-C6-O7
41	D	409	LHG	O9-C7-O7-C5
31	b	607	CLA	CBA-CGA-O2A-C1
41	D1	408	LHG	C24-C23-O8-C6
35	j	101	LMG	C11-C12-C13-C14
41	L	101	LHG	C35-C36-C37-C38
41	S1	624	LHG	C30-C31-C32-C33
54	I1	102	4RF	C32-C33-C34-C35
41	c	625	LHG	O10-C23-O8-C6
54	I1	102	4RF	O42-C41-O40-C39
31	c1	513	CLA	C16-C17-C18-C19
31	c	505	CLA	C5-C6-C7-C8
31	n	602	CLA	C10-C11-C12-C13
35	c1	521	LMG	C21-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	b	623	DGA	CA8-CA9-CAA-CBA
40	c	519	DGD	C5A-C6A-C7A-C8A
41	c	625	LHG	C35-C36-C37-C38
31	A1	405	CLA	CAA-CBA-CGA-O2A
40	C	519	DGD	C9A-CAA-CBA-CCA
41	D	409	LHG	C33-C34-C35-C36
53	Y1	625	SPH	C9-C10-C11-C12
54	k1	101	4RF	O42-C41-O40-C39
41	G	630	LHG	C10-C11-C12-C13
31	A	410	CLA	C3-C5-C6-C7
35	D1	411	LMG	C33-C34-C35-C36
41	s1	624	LHG	C33-C34-C35-C36
34	b	621	SQD	O47-C45-C46-O48
34	B1	626	SQD	O6-C44-C45-O47
34	a1	412	SQD	O47-C45-C46-O48
35	A	413	LMG	O7-C8-C9-O8
35	C	521	LMG	O1-C7-C8-O7
35	H	102	LMG	O7-C8-C9-O8
35	a	413	LMG	O7-C8-C9-O8
35	h	102	LMG	O7-C8-C9-O8
35	w1	201	LMG	O7-C8-C9-O8
40	C	519	DGD	O1G-C1G-C2G-O2G
41	C	525	LHG	O7-C5-C6-O8
41	C1	525	LHG	O7-C5-C6-O8
41	Y1	624	LHG	O7-C5-C6-O8
42	C	527	LMK	O1-C7-C8-O7
52	i	101	3PH	O21-C2-C3-O31
52	T1	101	3PH	O21-C2-C3-O31
54	K1	101	4RF	O21-C20-C39-O40
57	y1	627	PTY	O4-C1-C6-O7
40	c1	519	DGD	C2A-C1A-O1G-C1G
31	n	603	CLA	C13-C15-C16-C17
31	Y1	612	CLA	C8-C10-C11-C12
35	C1	521	LMG	O7-C10-C11-C12
41	c1	525	LHG	C30-C31-C32-C33
53	Y1	625	SPH	C6-C7-C8-C9
31	B	610	CLA	C16-C17-C18-C20
31	S1	603	CLA	C16-C17-C18-C19
34	A1	412	SQD	C30-C31-C32-C33
41	d1	410	LHG	C33-C34-C35-C36
34	C	526	SQD	O5-C1-O6-C44
34	M1	101	SQD	O5-C1-O6-C44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	W1	201	LMG	O6-C1-O1-C7
31	b	602	CLA	C8-C10-C11-C12
31	c	509	CLA	C10-C11-C12-C13
31	s	610	CLA	C8-C10-C11-C12
31	r1	612	CLA	C8-C10-C11-C12
38	c	524	DGA	CG1-CG2-CG3-OXT
38	c1	524	DGA	CG1-CG2-CG3-OXT
38	j1	101	DGA	CG1-CG2-CG3-OXT
41	S	624	LHG	C1-C2-C3-O3
41	n1	624	LHG	C1-C2-C3-O3
41	C	525	LHG	C31-C32-C33-C34
41	D1	409	LHG	C33-C34-C35-C36
41	G1	624	LHG	C9-C10-C11-C12
41	n1	624	LHG	C9-C10-C11-C12
54	k1	101	4RF	C10-C11-C12-C13
35	w1	201	LMG	O9-C10-O7-C8
41	c1	525	LHG	O9-C7-O7-C5
57	y1	626	PTY	O10-C8-O7-C6
57	y1	627	PTY	O30-C30-O4-C1
31	B	609	CLA	C4-C3-C5-C6
31	B	604	CLA	C2-C1-O2A-CGA
31	B	610	CLA	C2-C1-O2A-CGA
31	c	501	CLA	C2-C1-O2A-CGA
31	y	602	CLA	C2-C1-O2A-CGA
31	C1	501	CLA	C2-C1-O2A-CGA
47	R1	607	CHL	C2-C1-O2A-CGA
40	c	523	DGD	C7B-C8B-C9B-CAB
41	N1	624	LHG	C35-C36-C37-C38
41	y1	624	LHG	C35-C36-C37-C38
52	i	101	3PH	C39-C3A-C3B-C3C
31	Y	610	CLA	O1A-CGA-O2A-C1
31	r1	610	CLA	O1A-CGA-O2A-C1
32	a	408	PHO	O1A-CGA-O2A-C1
31	s1	603	CLA	C13-C15-C16-C17
31	B	606	CLA	C6-C7-C8-C9
31	B	613	CLA	C6-C7-C8-C9
31	B	615	CLA	C11-C12-C13-C14
31	B	617	CLA	C11-C12-C13-C14
31	C	506	CLA	C6-C7-C8-C9
31	D	403	CLA	C6-C7-C8-C9
31	G	603	CLA	C6-C7-C8-C9
31	G	603	CLA	C14-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	S	610	CLA	C11-C12-C13-C14
31	Y	602	CLA	C6-C7-C8-C9
31	Y	604	CLA	C11-C12-C13-C14
31	Y	613	CLA	C6-C7-C8-C9
31	c	506	CLA	C11-C10-C8-C9
31	c	506	CLA	C11-C12-C13-C14
31	c	509	CLA	C6-C7-C8-C9
31	g	602	CLA	C11-C10-C8-C9
31	s	603	CLA	C11-C10-C8-C9
31	y	613	CLA	C11-C10-C8-C9
31	B1	610	CLA	C6-C7-C8-C9
31	B1	614	CLA	C6-C7-C8-C9
31	D1	402	CLA	C11-C10-C8-C9
31	N1	613	CLA	C11-C12-C13-C14
31	G1	610	CLA	C6-C7-C8-C9
31	b1	604	CLA	C11-C10-C8-C9
31	b1	616	CLA	C11-C12-C13-C14
31	c1	507	CLA	C14-C13-C15-C16
31	c1	511	CLA	C11-C10-C8-C9
31	y1	612	CLA	C11-C10-C8-C9
32	A1	408	PHO	C6-C7-C8-C9
47	Y	609	CHL	C14-C13-C15-C16
47	n	605	CHL	C14-C13-C15-C16
47	g	601	CHL	C11-C12-C13-C14
47	y	609	CHL	C11-C12-C13-C14
47	N1	607	CHL	C11-C10-C8-C9
47	N1	607	CHL	C11-C12-C13-C14
47	y1	607	CHL	C6-C7-C8-C9
47	y1	607	CHL	C14-C13-C15-C16
53	Y	625	SPH	C14-C15-C16-C17
55	r1	625	LMT	C5-C6-C7-C8
38	b1	625	DGA	CB5-CB6-CB7-CB8
41	n	624	LHG	C35-C36-C37-C38
41	G1	624	LHG	C34-C35-C36-C37
41	d1	408	LHG	C24-C25-C26-C27
31	C	509	CLA	C15-C16-C17-C18
31	G	602	CLA	C5-C6-C7-C8
31	b	608	CLA	C10-C11-C12-C13
31	n	602	CLA	C15-C16-C17-C18
31	C1	513	CLA	C15-C16-C17-C18
31	c1	507	CLA	C13-C15-C16-C17
41	D	410	LHG	C2-C3-O3-P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	s	624	LHG	C2-C3-O3-P
41	L1	101	LHG	C2-C3-O3-P
41	d1	408	LHG	C2-C3-O3-P
41	d1	409	LHG	C2-C3-O3-P
41	s1	624	LHG	C2-C3-O3-P
53	y	625	SPH	O1-C1-C2-C3
38	B	625	DGA	CA6-CA7-CA8-CA9
41	d	409	LHG	C24-C25-C26-C27
31	R	608	CLA	C2A-CAA-CBA-CGA
31	N	604	CLA	C16-C17-C18-C19
31	r	603	CLA	C11-C12-C13-C15
40	C1	520	DGD	O6D-C5D-C6D-O5D
31	C	513	CLA	C3-C5-C6-C7
33	B	618	BCR	C23-C24-C25-C26
33	C	517	BCR	C23-C24-C25-C30
33	d	404	BCR	C23-C24-C25-C26
33	d	404	BCR	C23-C24-C25-C30
33	C1	515	BCR	C23-C24-C25-C30
37	B1	620	C7Z	C25-C26-C27-C28
48	R	620	LUT	C1-C6-C7-C8
48	R	620	LUT	C5-C6-C7-C8
48	Y	620	LUT	C1-C6-C7-C8
48	Y	620	LUT	C5-C6-C7-C8
48	n	620	LUT	C1-C6-C7-C8
48	n	620	LUT	C5-C6-C7-C8
48	r	620	LUT	C5-C6-C7-C8
48	N1	621	LUT	C1-C6-C7-C8
48	N1	621	LUT	C5-C6-C7-C8
48	G1	621	LUT	C1-C6-C7-C8
48	G1	621	LUT	C5-C6-C7-C8
48	S1	620	LUT	C5-C6-C7-C8
48	y1	621	LUT	C5-C6-C7-C8
31	D	403	CLA	C10-C11-C12-C13
31	s	609	CLA	C10-C11-C12-C13
31	y1	611	CLA	C10-C11-C12-C13
34	B	621	SQD	C16-C17-C18-C19
41	g1	624	LHG	C9-C10-C11-C12
52	B1	624	3PH	C3B-C3C-C3D-C3E
33	C1	514	BCR	C37-C22-C23-C24
37	B1	620	C7Z	C11-C12-C13-C20
44	d1	405	PL9	C47-C48-C49-C50
47	s1	606	CHL	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	a1	412	SQD	C28-C29-C30-C31
40	c1	520	DGD	C5A-C6A-C7A-C8A
33	b	619	BCR	C11-C12-C13-C14
33	c	515	BCR	C7-C8-C9-C10
33	B1	618	BCR	C21-C22-C23-C24
33	C1	514	BCR	C17-C18-C19-C20
33	C1	517	BCR	C7-C8-C9-C10
47	S	607	CHL	C1A-C2A-CAA-CBA
48	s1	620	LUT	C31-C32-C33-C34
49	Y	622	XAT	C27-C28-C29-C30
50	s	623	NEX	C11-C12-C13-C14
31	A	406	CLA	C10-C11-C12-C13
31	y	611	CLA	C5-C6-C7-C8
31	b1	609	CLA	C13-C15-C16-C17
54	il	101	4RF	C51-C52-C53-C54
40	c1	519	DGD	C1B-C2B-C3B-C4B
40	c1	519	DGD	O1B-C1B-O2G-C2G
49	N1	622	XAT	C14-C15-C35-C34
35	w1	201	LMG	C37-C38-C39-C40
41	N1	624	LHG	C24-C25-C26-C27
31	b1	613	CLA	C8-C10-C11-C12
40	c1	519	DGD	CCB-CDB-CEB-CFB
41	D1	409	LHG	C30-C31-C32-C33
31	n	610	CLA	C16-C17-C18-C19
31	Y1	610	CLA	C16-C17-C18-C20
47	S1	608	CHL	C11-C12-C13-C15
34	c1	526	SQD	C7-C8-C9-C10
54	il	101	4RF	C13-C14-C15-C16
31	n1	602	CLA	C8-C10-C11-C12
47	g	601	CHL	C10-C11-C12-C13
56	r1	626	ERG	C22-C23-C24-C28
31	G	610	CLA	O1A-CGA-O2A-C1
31	y	610	CLA	O1A-CGA-O2A-C1
42	c1	527	LMK	O8-C28-C29-C30
34	c	626	SQD	C15-C16-C17-C18
41	C1	525	LHG	C34-C35-C36-C37
31	C	511	CLA	C10-C11-C12-C13
31	g1	613	CLA	C13-C15-C16-C17
41	D	410	LHG	O6-C4-C5-C6
41	d	409	LHG	O6-C4-C5-C6
41	n1	624	LHG	O6-C4-C5-C6
52	s	626	3PH	O11-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
57	y1	627	PTY	O14-C5-C6-C1
31	n	613	CLA	C4-C3-C5-C6
47	Y1	609	CHL	C4-C3-C5-C6
52	S	626	3PH	C2E-C2F-C2G-C2H
54	I1	102	4RF	C12-C13-C14-C15
57	Y1	626	PTY	C20-C21-C22-C23
40	C	520	DGD	C4E-C5E-C6E-O5E
31	A	406	CLA	C11-C10-C8-C7
31	B	607	CLA	C6-C7-C8-C10
31	B	613	CLA	C6-C7-C8-C10
31	B	615	CLA	C11-C12-C13-C15
31	C	501	CLA	C11-C10-C8-C7
31	C	502	CLA	C11-C12-C13-C15
31	C	503	CLA	C11-C10-C8-C7
31	C	503	CLA	C12-C13-C15-C16
31	C	506	CLA	C12-C13-C15-C16
31	C	507	CLA	C11-C10-C8-C7
31	C	510	CLA	C6-C7-C8-C10
31	C	510	CLA	C11-C10-C8-C7
31	C	512	CLA	C11-C10-C8-C7
31	C	512	CLA	C12-C13-C15-C16
31	C	513	CLA	C11-C10-C8-C7
31	D	403	CLA	C6-C7-C8-C10
31	N	602	CLA	C11-C10-C8-C7
31	G	602	CLA	C6-C7-C8-C10
31	G	602	CLA	C12-C13-C15-C16
31	G	603	CLA	C12-C13-C15-C16
31	G	613	CLA	C11-C10-C8-C7
31	G	613	CLA	C12-C13-C15-C16
31	S	603	CLA	C11-C10-C8-C7
31	S	611	CLA	C12-C13-C15-C16
31	Y	602	CLA	C6-C7-C8-C10
31	Y	602	CLA	C11-C12-C13-C15
31	Y	604	CLA	C11-C12-C13-C15
31	b	604	CLA	C6-C7-C8-C10
31	b	608	CLA	C11-C12-C13-C15
31	b	615	CLA	C11-C12-C13-C15
31	b	617	CLA	C6-C7-C8-C10
31	c	508	CLA	C12-C13-C15-C16
31	c	512	CLA	C11-C10-C8-C7
31	c	512	CLA	C11-C12-C13-C15
31	c	512	CLA	C12-C13-C15-C16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	d	402	CLA	C11-C12-C13-C15
31	d	403	CLA	C11-C12-C13-C15
31	n	613	CLA	C2-C3-C5-C6
31	n	613	CLA	C12-C13-C15-C16
31	g	603	CLA	C11-C12-C13-C15
31	g	613	CLA	C12-C13-C15-C16
31	s	603	CLA	C11-C10-C8-C7
31	s	611	CLA	C11-C10-C8-C7
31	y	610	CLA	C6-C7-C8-C10
31	y	612	CLA	C11-C12-C13-C15
31	y	614	CLA	C11-C10-C8-C7
31	A1	406	CLA	C12-C13-C15-C16
31	B1	605	CLA	C11-C10-C8-C7
31	B1	608	CLA	C11-C12-C13-C15
31	B1	608	CLA	C12-C13-C15-C16
31	B1	609	CLA	C11-C12-C13-C15
31	B1	614	CLA	C6-C7-C8-C10
31	B1	616	CLA	C11-C10-C8-C7
31	B1	616	CLA	C11-C12-C13-C15
31	B1	617	CLA	C6-C7-C8-C10
31	C1	504	CLA	C11-C10-C8-C7
31	C1	505	CLA	C12-C13-C15-C16
31	C1	510	CLA	C2-C3-C5-C6
31	C1	510	CLA	C6-C7-C8-C10
31	C1	513	CLA	C11-C10-C8-C7
31	D1	402	CLA	C6-C7-C8-C10
31	D1	402	CLA	C11-C10-C8-C7
31	D1	403	CLA	C6-C7-C8-C10
31	G1	610	CLA	C6-C7-C8-C10
31	G1	610	CLA	C11-C12-C13-C15
31	G1	613	CLA	C12-C13-C15-C16
31	S1	610	CLA	C11-C10-C8-C7
31	S1	610	CLA	C11-C12-C13-C15
31	Y1	602	CLA	C6-C7-C8-C10
31	Y1	602	CLA	C11-C12-C13-C15
31	Y1	612	CLA	C11-C10-C8-C7
31	b1	616	CLA	C11-C12-C13-C15
31	c1	501	CLA	C12-C13-C15-C16
31	c1	503	CLA	C12-C13-C15-C16
31	c1	504	CLA	C11-C10-C8-C7
31	c1	505	CLA	C12-C13-C15-C16
31	c1	509	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c1	512	CLA	C11-C10-C8-C7
31	n1	602	CLA	C11-C10-C8-C7
31	n1	603	CLA	C12-C13-C15-C16
31	n1	613	CLA	C11-C10-C8-C7
31	g1	602	CLA	C6-C7-C8-C10
31	r1	608	CLA	C6-C7-C8-C10
31	r1	609	CLA	C11-C10-C8-C7
31	y1	602	CLA	C12-C13-C15-C16
31	y1	610	CLA	C11-C12-C13-C15
31	y1	613	CLA	C11-C10-C8-C7
47	N	605	CHL	C11-C10-C8-C7
47	N	605	CHL	C12-C13-C15-C16
47	N	607	CHL	C11-C10-C8-C7
47	Y	609	CHL	C12-C13-C15-C16
47	n	607	CHL	C12-C13-C15-C16
47	g	601	CHL	C11-C12-C13-C15
47	y	601	CHL	C11-C10-C8-C7
47	y	606	CHL	C11-C10-C8-C7
47	N1	601	CHL	C12-C13-C15-C16
47	N1	605	CHL	C11-C10-C8-C7
47	N1	605	CHL	C11-C12-C13-C15
47	N1	606	CHL	C11-C10-C8-C7
47	N1	606	CHL	C11-C12-C13-C15
47	N1	607	CHL	C11-C10-C8-C7
47	G1	607	CHL	C11-C10-C8-C7
47	G1	609	CHL	C11-C12-C13-C15
47	Y1	606	CHL	C6-C7-C8-C10
47	Y1	607	CHL	C11-C10-C8-C7
47	n1	601	CHL	C12-C13-C15-C16
47	n1	606	CHL	C11-C12-C13-C15
47	g1	601	CHL	C6-C7-C8-C10
31	g	613	CLA	C3-C5-C6-C7
31	s1	609	CLA	O1A-CGA-O2A-C1
34	a	412	SQD	C34-C35-C36-C37
41	L	101	LHG	C34-C35-C36-C37
38	j1	101	DGA	OG2-CG2-CG3-OXT
31	n	602	CLA	C8-C10-C11-C12
33	C	515	BCR	C19-C20-C21-C22
33	b	619	BCR	C9-C10-C11-C12
33	D1	404	BCR	C9-C10-C11-C12
33	d1	404	BCR	C13-C14-C15-C16
37	B	620	C7Z	C29-C30-C31-C32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
37	b1	620	C7Z	C33-C34-C35-C15
46	h1	101	RRX	C19-C20-C21-C22
48	R	620	LUT	C13-C14-C15-C35
48	R	620	LUT	C33-C34-C35-C15
48	g	621	LUT	C29-C30-C31-C32
48	R1	620	LUT	C33-C34-C35-C15
48	n1	620	LUT	C9-C10-C11-C12
49	y	622	XAT	C29-C30-C31-C32
31	b	613	CLA	C16-C17-C18-C19
31	Y1	611	CLA	C16-C17-C18-C20
41	g	624	LHG	C35-C36-C37-C38
35	A1	413	LMG	C34-C35-C36-C37
40	C1	520	DGD	C3B-C4B-C5B-C6B
41	g1	624	LHG	C26-C27-C28-C29
31	c	505	CLA	C15-C16-C17-C18
31	D1	403	CLA	C5-C6-C7-C8
31	S1	602	CLA	C5-C6-C7-C8
35	H	102	LMG	O7-C10-C11-C12
31	G	602	CLA	C2A-CAA-CBA-CGA
31	g1	610	CLA	C2A-CAA-CBA-CGA
34	b1	621	SQD	C13-C14-C15-C16
41	d	410	LHG	C30-C31-C32-C33
52	b1	624	3PH	C22-C23-C24-C25
40	c1	519	DGD	C2B-C1B-O2G-C2G
42	C	527	LMK	O1-C1-C2-C3
31	c	503	CLA	C5-C6-C7-C8
31	d	403	CLA	C8-C10-C11-C12
34	C1	526	SQD	C9-C10-C11-C12
34	b1	626	SQD	C29-C30-C31-C32
40	c	520	DGD	CCB-CDB-CEB-CFB
50	N	623	NEX	C20-C13-C14-C15
50	n	623	NEX	C11-C10-C9-C19
50	r	623	NEX	C40-C33-C34-C35
50	n1	623	NEX	C20-C13-C14-C15
50	s1	623	NEX	C40-C33-C34-C35
35	B1	622	LMG	C10-C11-C12-C13
31	a	406	CLA	C3-C5-C6-C7
31	b	613	CLA	C3-C5-C6-C7
31	c	501	CLA	C3-C5-C6-C7
31	B1	607	CLA	C3-C5-C6-C7
31	D1	403	CLA	C16-C17-C18-C19
31	B1	606	CLA	C13-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
32	A1	409	PHO	CBA-CGA-O2A-C1
31	R	609	CLA	CAA-CBA-CGA-O2A
47	n	607	CHL	CAA-CBA-CGA-O2A
53	A1	414	SPH	C15-C16-C17-C18
55	R1	625	LMT	C4'-C5'-C6'-O6'
34	c	626	SQD	C7-C8-C9-C10
41	S1	624	LHG	C35-C36-C37-C38
51	s1	625	LPX	C9-C10-C11-C12
31	y	612	CLA	C8-C10-C11-C12
31	A	410	CLA	CAD-CBD-CGD-O2D
31	B	605	CLA	CAD-CBD-CGD-O2D
31	B	612	CLA	CAD-CBD-CGD-O2D
31	B	617	CLA	CAD-CBD-CGD-O2D
31	C	503	CLA	CAD-CBD-CGD-O2D
31	C	505	CLA	CAD-CBD-CGD-O2D
31	N	603	CLA	CAD-CBD-CGD-O2D
31	b	608	CLA	CAD-CBD-CGD-O2D
31	c	510	CLA	CAD-CBD-CGD-O2D
31	n	603	CLA	CAD-CBD-CGD-O2D
31	n	612	CLA	CAD-CBD-CGD-O2D
31	s	611	CLA	CAD-CBD-CGD-O2D
31	y	614	CLA	CAD-CBD-CGD-O2D
31	C1	506	CLA	CAD-CBD-CGD-O2D
31	C1	510	CLA	CAD-CBD-CGD-O2D
31	G1	604	CLA	CAD-CBD-CGD-O2D
31	c1	501	CLA	CAD-CBD-CGD-O2D
31	c1	503	CLA	CAD-CBD-CGD-O2D
31	c1	504	CLA	CAD-CBD-CGD-O2D
31	c1	506	CLA	CAD-CBD-CGD-O2D
31	n1	602	CLA	CAD-CBD-CGD-O2D
31	n1	611	CLA	CAD-CBD-CGD-O2D
31	y1	603	CLA	CAD-CBD-CGD-O2D
34	B1	621	SQD	C46-C45-O47-C7
34	b1	621	SQD	C46-C45-O47-C7
34	m1	101	SQD	C46-C45-O47-C7
38	B	625	DGA	CG1-CG2-OG2-CB1
38	B1	625	DGA	CG1-CG2-OG2-CB1
40	C	523	DGD	C1G-C2G-O2G-C1B
47	N	607	CHL	CAD-CBD-CGD-O2D
47	g	606	CHL	CAD-CBD-CGD-O2D
47	s	606	CHL	CAD-CBD-CGD-O2D
47	y	605	CHL	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	S1	606	CHL	CAD-CBD-CGD-O2D
47	g1	606	CHL	CAD-CBD-CGD-O2D
50	S	622	NEX	C7-C8-C9-C19
50	s	623	NEX	C7-C8-C9-C19
50	N1	623	NEX	C7-C8-C9-C19
41	D1	409	LHG	C13-C14-C15-C16
52	s	626	3PH	C26-C27-C28-C29
31	C	510	CLA	C8-C10-C11-C12
31	b	605	CLA	C5-C6-C7-C8
35	H	102	LMG	C19-C20-C21-C22
40	c	520	DGD	C3B-C4B-C5B-C6B
31	N	604	CLA	CBA-CGA-O2A-C1
31	B1	605	CLA	CBA-CGA-O2A-C1
31	B	602	CLA	C4-C3-C5-C6
31	C1	509	CLA	C4-C3-C5-C6
47	N	609	CHL	C4-C3-C5-C6
31	B	602	CLA	C16-C17-C18-C20
31	B	612	CLA	C16-C17-C18-C19
31	Y	613	CLA	C16-C17-C18-C20
31	B1	607	CLA	C16-C17-C18-C20
31	n1	613	CLA	C16-C17-C18-C19
38	c	524	DGA	CA6-CA7-CA8-CA9
40	c	519	DGD	O6D-C1D-O3G-C3G
31	D	403	CLA	C13-C15-C16-C17
31	c	510	CLA	C8-C10-C11-C12
31	n	610	CLA	C8-C10-C11-C12
31	B	602	CLA	C2-C3-C5-C6
47	Y1	609	CHL	C2-C3-C5-C6
41	G	630	LHG	C11-C10-C9-C8
34	A	412	SQD	C44-C45-C46-O48
34	C1	526	SQD	O6-C44-C45-C46
38	C1	524	DGA	OG1-CG1-CG2-CG3
40	c1	519	DGD	O1G-C1G-C2G-C3G
41	S	624	LHG	C2-C3-O3-P
41	S	624	LHG	C4-C5-C6-O8
41	Y	624	LHG	C4-C5-C6-O8
41	c	625	LHG	C4-C5-C6-O8
41	s	624	LHG	C4-C5-C6-O8
41	c1	525	LHG	C2-C3-O3-P
41	d1	410	LHG	C2-C3-O3-P
41	n1	624	LHG	C4-C5-C6-O8
42	c1	527	LMK	C11-C10-O7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
52	s	626	3PH	C1-C2-C3-O31
54	i1	101	4RF	O18-C19-C20-C39
57	Y1	627	PTY	O4-C1-C6-C5
57	y1	626	PTY	O4-C1-C6-C5
34	b1	621	SQD	O10-C23-O48-C46
41	C	525	LHG	O6-C4-C5-O7
41	G	630	LHG	O6-C4-C5-O7
41	d	408	LHG	O6-C4-C5-O7
41	C1	525	LHG	O6-C4-C5-O7
41	L1	101	LHG	O6-C4-C5-O7
41	d1	408	LHG	O6-C4-C5-O7
52	i	101	3PH	O11-C1-C2-O21
57	y1	626	PTY	O14-C5-C6-O7
31	S	614	CLA	C5-C6-C7-C8
31	Y1	613	CLA	C13-C15-C16-C17
31	b1	606	CLA	C10-C11-C12-C13
31	r1	602	CLA	C3-C5-C6-C7
41	L	101	LHG	O7-C7-C8-C9
41	n1	624	LHG	O8-C23-C24-C25
31	C1	505	CLA	O1D-CGD-O2D-CED
52	B1	624	3PH	C2E-C2F-C2G-C2H
45	F	101	HEM	C4B-C3B-CAB-CBB
31	C	506	CLA	C2A-CAA-CBA-CGA
38	C	524	DGA	CBB-CCB-CDB-CEB
41	G	630	LHG	C16-C17-C18-C19
41	S1	624	LHG	C13-C14-C15-C16
31	d	402	CLA	C16-C17-C18-C19
35	j	101	LMG	C30-C31-C32-C33
38	C1	524	DGA	CAB-CBB-CCB-CDB
41	D	409	LHG	C16-C17-C18-C19
41	Y1	624	LHG	C9-C10-C11-C12
31	B	609	CLA	CHA-CBD-CGD-O1D
31	B	609	CLA	CHA-CBD-CGD-O2D
31	C	501	CLA	CHA-CBD-CGD-O1D
31	C	501	CLA	CHA-CBD-CGD-O2D
31	G	602	CLA	CHA-CBD-CGD-O1D
31	G	602	CLA	CHA-CBD-CGD-O2D
31	G	612	CLA	CHA-CBD-CGD-O1D
31	G	612	CLA	CHA-CBD-CGD-O2D
31	R	603	CLA	CHA-CBD-CGD-O1D
31	R	603	CLA	CHA-CBD-CGD-O2D
31	R	604	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	604	CLA	CHA-CBD-CGD-O2D
31	R	609	CLA	CHA-CBD-CGD-O1D
31	R	612	CLA	CHA-CBD-CGD-O1D
31	R	612	CLA	CHA-CBD-CGD-O2D
31	R	613	CLA	CHA-CBD-CGD-O1D
31	R	613	CLA	CHA-CBD-CGD-O2D
31	Y	612	CLA	CHA-CBD-CGD-O1D
31	Y	612	CLA	CHA-CBD-CGD-O2D
31	b	606	CLA	CHA-CBD-CGD-O1D
31	b	610	CLA	CHA-CBD-CGD-O2D
31	b	611	CLA	CHA-CBD-CGD-O1D
31	b	611	CLA	CHA-CBD-CGD-O2D
31	b	613	CLA	CHA-CBD-CGD-O1D
31	c	501	CLA	CHA-CBD-CGD-O1D
31	c	502	CLA	CHA-CBD-CGD-O1D
31	c	503	CLA	CHA-CBD-CGD-O1D
31	c	504	CLA	CHA-CBD-CGD-O1D
31	c	504	CLA	CHA-CBD-CGD-O2D
31	n	610	CLA	CHA-CBD-CGD-O1D
31	n	610	CLA	CHA-CBD-CGD-O2D
31	r	602	CLA	CHA-CBD-CGD-O1D
31	r	602	CLA	CHA-CBD-CGD-O2D
31	r	612	CLA	CHA-CBD-CGD-O1D
31	r	612	CLA	CHA-CBD-CGD-O2D
31	r	613	CLA	CHA-CBD-CGD-O1D
31	r	613	CLA	CHA-CBD-CGD-O2D
31	s	612	CLA	CHA-CBD-CGD-O1D
31	s	612	CLA	CHA-CBD-CGD-O2D
31	s	613	CLA	CHA-CBD-CGD-O1D
31	y	611	CLA	CHA-CBD-CGD-O1D
31	y	611	CLA	CHA-CBD-CGD-O2D
31	y	612	CLA	CHA-CBD-CGD-O1D
31	y	612	CLA	CHA-CBD-CGD-O2D
31	A1	407	CLA	CHA-CBD-CGD-O1D
31	A1	407	CLA	CHA-CBD-CGD-O2D
31	B1	603	CLA	CHA-CBD-CGD-O2D
31	B1	605	CLA	CHA-CBD-CGD-O2D
31	B1	617	CLA	CHA-CBD-CGD-O1D
31	B1	617	CLA	CHA-CBD-CGD-O2D
31	C1	502	CLA	CHA-CBD-CGD-O2D
31	C1	503	CLA	CHA-CBD-CGD-O1D
31	C1	503	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N1	604	CLA	CHA-CBD-CGD-O1D
31	N1	610	CLA	CHA-CBD-CGD-O1D
31	N1	610	CLA	CHA-CBD-CGD-O2D
31	N1	612	CLA	CHA-CBD-CGD-O1D
31	N1	612	CLA	CHA-CBD-CGD-O2D
31	G1	612	CLA	CHA-CBD-CGD-O1D
31	G1	612	CLA	CHA-CBD-CGD-O2D
31	R1	602	CLA	CHA-CBD-CGD-O1D
31	R1	603	CLA	CHA-CBD-CGD-O1D
31	R1	603	CLA	CHA-CBD-CGD-O2D
31	R1	604	CLA	CHA-CBD-CGD-O2D
31	R1	608	CLA	CHA-CBD-CGD-O1D
31	R1	608	CLA	CHA-CBD-CGD-O2D
31	S1	602	CLA	CHA-CBD-CGD-O1D
31	S1	602	CLA	CHA-CBD-CGD-O2D
31	S1	603	CLA	CHA-CBD-CGD-O1D
31	S1	603	CLA	CHA-CBD-CGD-O2D
31	S1	610	CLA	CHA-CBD-CGD-O1D
31	S1	610	CLA	CHA-CBD-CGD-O2D
31	S1	611	CLA	CHA-CBD-CGD-O1D
31	S1	612	CLA	CHA-CBD-CGD-O1D
31	S1	612	CLA	CHA-CBD-CGD-O2D
31	Y1	612	CLA	CHA-CBD-CGD-O1D
31	Y1	612	CLA	CHA-CBD-CGD-O2D
31	b1	607	CLA	CHA-CBD-CGD-O1D
31	b1	607	CLA	CHA-CBD-CGD-O2D
31	c1	507	CLA	CHA-CBD-CGD-O1D
31	c1	507	CLA	CHA-CBD-CGD-O2D
31	c1	509	CLA	CHA-CBD-CGD-O1D
31	c1	509	CLA	CHA-CBD-CGD-O2D
31	n1	604	CLA	CHA-CBD-CGD-O2D
31	n1	612	CLA	CHA-CBD-CGD-O1D
31	n1	613	CLA	CHA-CBD-CGD-O1D
31	g1	610	CLA	CHA-CBD-CGD-O2D
31	g1	611	CLA	CHA-CBD-CGD-O2D
31	g1	612	CLA	CHA-CBD-CGD-O1D
31	g1	612	CLA	CHA-CBD-CGD-O2D
31	r1	602	CLA	CHA-CBD-CGD-O1D
31	r1	602	CLA	CHA-CBD-CGD-O2D
31	s1	602	CLA	CHA-CBD-CGD-O1D
31	s1	604	CLA	CHA-CBD-CGD-O1D
31	s1	604	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s1	605	CLA	CHA-CBD-CGD-O2D
33	C	516	BCR	C9-C10-C11-C12
42	c	627	LMK	C2-C3-C4-O2
47	n1	601	CHL	CHA-CBD-CGD-O1D
47	n1	601	CHL	CHA-CBD-CGD-O2D
47	r1	606	CHL	CHA-CBD-CGD-O1D
47	r1	606	CHL	CHA-CBD-CGD-O2D
47	s1	606	CHL	CHA-CBD-CGD-O2D
47	y1	607	CHL	CHA-CBD-CGD-O2D
35	B1	622	LMG	C14-C15-C16-C17
31	S	614	CLA	O1A-CGA-O2A-C1
31	b	607	CLA	O1A-CGA-O2A-C1
31	s	604	CLA	O1A-CGA-O2A-C1
31	A1	405	CLA	O1A-CGA-O2A-C1
31	G1	610	CLA	O1A-CGA-O2A-C1
31	n1	610	CLA	O1A-CGA-O2A-C1
32	A1	408	PHO	O1A-CGA-O2A-C1
38	C1	524	DGA	OA1-CA1-OG1-CG1
38	j1	101	DGA	OA1-CA1-OG1-CG1
41	d1	408	LHG	O10-C23-O8-C6
40	c	519	DGD	C9A-CAA-CBA-CCA
40	C1	518	DGD	C3B-C4B-C5B-C6B
41	L	101	LHG	C29-C30-C31-C32
51	S	625	LPX	C14-C15-C16-C17
31	r1	608	CLA	C5-C6-C7-C8
34	C1	526	SQD	O6-C44-C45-O47
34	a1	412	SQD	O6-C44-C45-O47
34	b1	626	SQD	O6-C44-C45-O47
34	c1	526	SQD	O6-C44-C45-O47
35	b	622	LMG	O7-C8-C9-O8
35	B1	622	LMG	O1-C7-C8-O7
35	C1	521	LMG	O7-C8-C9-O8
40	C	523	DGD	O1G-C1G-C2G-O2G
41	D	410	LHG	O7-C5-C6-O8
41	S	624	LHG	O7-C5-C6-O8
41	n	624	LHG	O7-C5-C6-O8
41	L1	101	LHG	O7-C5-C6-O8
41	c1	525	LHG	O7-C5-C6-O8
41	s1	624	LHG	O7-C5-C6-O8
52	s1	626	3PH	O21-C2-C3-O31
54	I1	102	4RF	O18-C19-C20-O21
57	Y1	627	PTY	O4-C1-C6-O7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	b1	626	SQD	C9-C10-C11-C12
52	i	101	3PH	C24-C25-C26-C27
53	y	625	SPH	C11-C12-C13-C14
31	y	604	CLA	C13-C15-C16-C17
31	b1	616	CLA	C8-C10-C11-C12
31	B1	612	CLA	O1A-CGA-O2A-C1
31	c1	502	CLA	O1A-CGA-O2A-C1
38	B1	625	DGA	CFA-CGA-CHA-CIA
41	g1	624	LHG	C24-C25-C26-C27
54	I1	102	4RF	C27-C28-C29-C30
54	k1	101	4RF	C01-C02-C03-C04
41	d	410	LHG	O1-C1-C2-O2
41	n1	624	LHG	O1-C1-C2-O2
53	Y	625	SPH	N2-C2-C3-O3
53	A1	414	SPH	N2-C2-C3-O3
40	c1	518	DGD	O6D-C5D-C6D-O5D
34	c1	526	SQD	C31-C32-C33-C34
38	C1	524	DGA	CB3-CB4-CB5-CB6
52	B1	624	3PH	C25-C26-C27-C28
31	b1	604	CLA	C3-C5-C6-C7
47	n	609	CHL	C8-C10-C11-C12
31	C	506	CLA	C4-C3-C5-C6
31	r	609	CLA	C4-C3-C5-C6
31	n1	604	CLA	C4-C3-C5-C6
31	y1	611	CLA	C4-C3-C5-C6
44	d1	405	PL9	C30-C29-C31-C32
40	c1	519	DGD	O1A-C1A-O1G-C1G
40	c	520	DGD	C2B-C3B-C4B-C5B
35	a1	413	LMG	O9-C10-O7-C8
40	C1	520	DGD	O1B-C1B-O2G-C2G
31	B	609	CLA	C11-C12-C13-C14
31	C	506	CLA	C14-C13-C15-C16
31	C	510	CLA	C11-C10-C8-C9
31	C	512	CLA	C14-C13-C15-C16
31	C	513	CLA	C11-C12-C13-C14
31	G	613	CLA	C11-C10-C8-C9
31	S	611	CLA	C14-C13-C15-C16
31	Y	614	CLA	C11-C10-C8-C9
31	b	604	CLA	C6-C7-C8-C9
31	b	608	CLA	C11-C12-C13-C14
31	d	402	CLA	C11-C12-C13-C14
31	d	403	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s	611	CLA	C11-C10-C8-C9
31	B1	608	CLA	C11-C12-C13-C14
31	B1	609	CLA	C11-C12-C13-C14
31	B1	617	CLA	C6-C7-C8-C9
31	c1	503	CLA	C6-C7-C8-C9
31	c1	504	CLA	C11-C10-C8-C9
31	r1	608	CLA	C6-C7-C8-C9
47	N	607	CHL	C11-C10-C8-C9
47	G1	601	CHL	C6-C7-C8-C9
47	Y1	609	CHL	C14-C13-C15-C16
47	g1	601	CHL	C6-C7-C8-C9
47	y1	609	CHL	C14-C13-C15-C16
40	c	519	DGD	C4D-C5D-C6D-O5D
35	c	521	LMG	C33-C34-C35-C36
38	J1	101	DGA	CA2-CA3-CA4-CA5
41	S	624	LHG	C10-C11-C12-C13
41	N1	624	LHG	C18-C19-C20-C21
41	D1	408	LHG	O10-C23-O8-C6
52	S1	626	3PH	C2C-C2D-C2E-C2F
31	B	617	CLA	C10-C11-C12-C13
47	G1	601	CHL	C5-C6-C7-C8
34	B	621	SQD	C4-C5-C6-S
34	C	526	SQD	C4-C5-C6-S
34	c	626	SQD	C4-C5-C6-S
34	C1	526	SQD	C5-C6-S-O8
34	m1	101	SQD	C4-C5-C6-S
31	B	610	CLA	C16-C17-C18-C19
31	b	615	CLA	C16-C17-C18-C19
34	B1	626	SQD	C24-C25-C26-C27
41	y	624	LHG	C35-C36-C37-C38
41	d1	409	LHG	C33-C34-C35-C36
54	k1	101	4RF	C26-C27-C28-C29
31	r1	603	CLA	C2A-CAA-CBA-CGA
47	R1	607	CHL	C2A-CAA-CBA-CGA
47	N1	608	CHL	CBD-CGD-O2D-CED
31	B	604	CLA	C15-C16-C17-C18
31	R	612	CLA	C5-C6-C7-C8
31	b1	615	CLA	C5-C6-C7-C8
35	D	411	LMG	C19-C20-C21-C22
32	A1	409	PHO	O1A-CGA-O2A-C1
33	C	516	BCR	C11-C12-C13-C35
33	A1	411	BCR	C7-C8-C9-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	c1	517	BCR	C37-C22-C23-C24
41	D	410	LHG	C30-C31-C32-C33
41	n1	624	LHG	O1-C1-C2-C3
40	C	520	DGD	O6E-C5E-C6E-O5E
31	G	610	CLA	C15-C16-C17-C18
34	b	621	SQD	C17-C18-C19-C20
38	B1	625	DGA	CA2-CA3-CA4-CA5
38	J1	101	DGA	CBB-CAB-CB9-CB8
33	c1	517	BCR	C21-C22-C23-C24
48	G1	620	LUT	C27-C28-C29-C30
49	n1	622	XAT	C31-C32-C33-C34
34	b1	626	SQD	C28-C29-C30-C31
40	c	520	DGD	C6B-C7B-C8B-C9B
53	Y1	625	SPH	C15-C16-C17-C18
54	K1	101	4RF	C01-C02-C03-C04
31	N	602	CLA	C1A-C2A-CAA-CBA
31	N	611	CLA	C1A-C2A-CAA-CBA
31	R	604	CLA	C1A-C2A-CAA-CBA
31	r	603	CLA	C1A-C2A-CAA-CBA
31	r	611	CLA	C1A-C2A-CAA-CBA
31	B1	605	CLA	C1A-C2A-CAA-CBA
31	D1	402	CLA	C1A-C2A-CAA-CBA
31	D1	403	CLA	C1A-C2A-CAA-CBA
31	G1	604	CLA	C1A-C2A-CAA-CBA
31	Y1	604	CLA	C1A-C2A-CAA-CBA
31	b1	605	CLA	C1A-C2A-CAA-CBA
31	g1	614	CLA	C1A-C2A-CAA-CBA
31	y1	608	CLA	C1A-C2A-CAA-CBA
47	N	609	CHL	C1A-C2A-CAA-CBA
47	G1	607	CHL	C1A-C2A-CAA-CBA
47	n1	607	CHL	C1A-C2A-CAA-CBA
35	w1	201	LMG	C28-C29-C30-C31
41	S	624	LHG	C7-C8-C9-C10
31	c	508	CLA	C16-C17-C18-C20
40	C1	520	DGD	C2B-C1B-O2G-C2G
31	B	616	CLA	C2-C1-O2A-CGA
31	G	603	CLA	C2-C1-O2A-CGA
31	a	405	CLA	C2-C1-O2A-CGA
31	c	507	CLA	C2-C1-O2A-CGA
31	c	513	CLA	C2-C1-O2A-CGA
31	n	611	CLA	C2-C1-O2A-CGA
31	s	609	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N1	614	CLA	C2-C1-O2A-CGA
31	G1	614	CLA	C2-C1-O2A-CGA
31	b1	607	CLA	C2-C1-O2A-CGA
31	n1	610	CLA	C2-C1-O2A-CGA
38	c	524	DGA	CA4-CA5-CA6-CA7
41	D	408	LHG	C25-C26-C27-C28
41	d	408	LHG	C24-C25-C26-C27
41	Y1	624	LHG	C11-C12-C13-C14
54	k1	101	4RF	C45-C46-C47-C48
33	b	619	BCR	C13-C14-C15-C16
33	c	515	BCR	C9-C10-C11-C12
48	r	620	LUT	C9-C10-C11-C12
31	n	604	CLA	O1D-CGD-O2D-CED
31	r	612	CLA	C5-C6-C7-C8
31	C1	501	CLA	C8-C10-C11-C12
41	N	624	LHG	C4-O6-P-O3
41	D1	409	LHG	C3-O3-P-O6
41	c1	525	LHG	C3-O3-P-O6
51	S1	625	LPX	C3-O1-P1-O2
51	s1	625	LPX	C1-O2-P1-O1
57	Y1	626	PTY	C5-O14-P1-O11
57	Y1	627	PTY	C3-O11-P1-O14
34	b1	621	SQD	C11-C10-C9-C8
41	D	409	LHG	C24-C25-C26-C27
35	W1	201	LMG	C29-C30-C31-C32
40	C	520	DGD	C7B-C8B-C9B-CAB
41	C1	525	LHG	C14-C15-C16-C17
54	I1	102	4RF	C46-C47-C48-C49
31	B	610	CLA	C4-C3-C5-C6
31	b	605	CLA	C4-C3-C5-C6
31	b	614	CLA	C4-C3-C5-C6
31	r	603	CLA	C4-C3-C5-C6
31	s1	603	CLA	C4-C3-C5-C6
41	D	409	LHG	C2-C3-O3-P
41	d	409	LHG	C2-C3-O3-P
41	S1	624	LHG	C2-C3-O3-P
52	s	626	3PH	C2-C1-O11-P
31	c	510	CLA	C2-C3-C5-C6
31	n1	610	CLA	C2-C3-C5-C6
38	C1	524	DGA	CB6-CB7-CB8-CB9
41	d1	410	LHG	C25-C26-C27-C28
52	s	626	3PH	C3E-C3F-C3G-C3H

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	N	604	CLA	O1A-CGA-O2A-C1
31	s	610	CLA	O1A-CGA-O2A-C1
31	B1	605	CLA	O1A-CGA-O2A-C1
41	C	525	LHG	C4-O6-P-O4
41	D	408	LHG	C4-O6-P-O4
41	D	409	LHG	C3-O3-P-O5
41	D	410	LHG	C4-O6-P-O4
41	S	624	LHG	C4-O6-P-O5
41	d	408	LHG	C4-O6-P-O4
41	d	410	LHG	C4-O6-P-O4
41	l	101	LHG	C3-O3-P-O5
41	n	624	LHG	C4-O6-P-O4
41	s	624	LHG	C4-O6-P-O5
41	y	624	LHG	C3-O3-P-O5
41	y	624	LHG	C4-O6-P-O4
41	C1	525	LHG	C3-O3-P-O4
41	D1	408	LHG	C3-O3-P-O5
41	D1	408	LHG	C4-O6-P-O4
41	L1	101	LHG	C3-O3-P-O5
41	N1	624	LHG	C4-O6-P-O4
41	G1	624	LHG	C3-O3-P-O5
41	d1	409	LHG	C4-O6-P-O4
41	d1	410	LHG	C3-O3-P-O4
51	S	625	LPX	C1-O2-P1-O4
51	s	625	LPX	C3-O1-P1-O3
51	s	625	LPX	C1-O2-P1-O4
57	y1	626	PTY	C5-O14-P1-O12
31	B	605	CLA	C16-C17-C18-C19
31	C	502	CLA	C16-C17-C18-C19
31	r	603	CLA	C11-C12-C13-C14
31	b1	617	CLA	C16-C17-C18-C20
40	C1	519	DGD	C1B-C2B-C3B-C4B
38	C1	524	DGA	CDA-CEA-CFA-CGA
41	d1	409	LHG	C30-C31-C32-C33
31	S	610	CLA	C13-C15-C16-C17
34	A1	412	SQD	C24-C23-O48-C46
38	C	524	DGA	CA2-CA1-OG1-CG1
40	B1	623	DGD	C2A-C1A-O1G-C1G
41	N	624	LHG	O6-C4-C5-C6
41	C1	525	LHG	C25-C26-C27-C28
34	b1	621	SQD	C24-C25-C26-C27
31	y	613	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b1	614	CLA	C2A-CAA-CBA-CGA
31	c1	501	CLA	C2A-CAA-CBA-CGA
32	a1	408	PHO	C2A-CAA-CBA-CGA
47	r1	607	CHL	C2A-CAA-CBA-CGA
31	A	406	CLA	C3-C5-C6-C7
31	B	604	CLA	C3-C5-C6-C7
31	c	508	CLA	C3-C5-C6-C7
40	C1	518	DGD	C4A-C5A-C6A-C7A
41	d	409	LHG	C19-C20-C21-C22
41	D1	408	LHG	C10-C11-C12-C13
41	D	409	LHG	C17-C18-C19-C20
52	T1	101	3PH	C3D-C3E-C3F-C3G
31	c	505	CLA	C16-C17-C18-C20
35	c1	521	LMG	C29-C30-C31-C32
41	D1	408	LHG	C31-C32-C33-C34
31	B	610	CLA	CAD-CBD-CGD-O1D
31	C	504	CLA	CAD-CBD-CGD-O1D
31	b	605	CLA	CAD-CBD-CGD-O1D
31	b	606	CLA	CAD-CBD-CGD-O1D
31	b	610	CLA	CAD-CBD-CGD-O1D
31	b	613	CLA	CAD-CBD-CGD-O1D
31	c	503	CLA	CAD-CBD-CGD-O1D
31	c	504	CLA	CAD-CBD-CGD-O1D
31	B1	608	CLA	CAD-CBD-CGD-O1D
31	C1	502	CLA	CAD-CBD-CGD-O1D
31	C1	503	CLA	CAD-CBD-CGD-O1D
31	N1	604	CLA	CAD-CBD-CGD-O1D
31	b1	605	CLA	CAD-CBD-CGD-O1D
31	n1	604	CLA	CAD-CBD-CGD-O1D
31	g1	604	CLA	CAD-CBD-CGD-O1D
34	C1	526	SQD	C5-C6-S-O7
34	M1	101	SQD	O5-C5-C6-S
47	S	601	CHL	CAD-CBD-CGD-O1D
47	s	601	CHL	CAD-CBD-CGD-O1D
47	n1	601	CHL	CAD-CBD-CGD-O1D
50	R	622	NEX	C7-C8-C9-C10
50	S	622	NEX	C7-C8-C9-C10
50	s	623	NEX	C7-C8-C9-C10
50	N1	623	NEX	C7-C8-C9-C10
50	y1	623	NEX	C7-C8-C9-C10
51	S	625	LPX	C2-C1-O2-P1
57	Y1	626	PTY	C2-C3-O11-P1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	B	625	DGA	CB1-CB2-CB3-CB4
31	S1	614	CLA	CAA-CBA-CGA-O2A
35	A1	413	LMG	O7-C10-C11-C12
31	N	603	CLA	C8-C10-C11-C12
31	c1	505	CLA	C15-C16-C17-C18
40	C	518	DGD	C5B-C6B-C7B-C8B
41	D1	409	LHG	C9-C10-C11-C12
41	N	624	LHG	C34-C35-C36-C37
41	L1	101	LHG	C12-C13-C14-C15
31	a	405	CLA	C8-C10-C11-C12
31	a	410	CLA	C5-C6-C7-C8
34	c1	526	SQD	C11-C10-C9-C8
35	A1	413	LMG	C12-C13-C14-C15
41	d	410	LHG	C28-C29-C30-C31
54	i1	101	4RF	C01-C02-C03-C04
38	b	623	DGA	CFB-CGB-CHB-CIB
41	d1	409	LHG	C24-C23-O8-C6
41	D	410	LHG	C1-C2-C3-O3
41	d1	408	LHG	C1-C2-C3-O3
53	y	625	SPH	C6-C7-C8-C9
54	I1	102	4RF	C10-C11-C12-C13
31	n	613	CLA	C16-C17-C18-C19
31	B	609	CLA	C11-C12-C13-C15
31	C	513	CLA	C11-C12-C13-C15
31	N	610	CLA	C11-C12-C13-C15
31	R	608	CLA	C6-C7-C8-C10
31	Y	604	CLA	C6-C7-C8-C10
31	Y	610	CLA	C6-C7-C8-C10
31	Y	614	CLA	C11-C10-C8-C7
31	a	405	CLA	C6-C7-C8-C10
31	b	605	CLA	C11-C12-C13-C15
31	c	501	CLA	C11-C10-C8-C7
31	c	508	CLA	C11-C10-C8-C7
31	c	513	CLA	C11-C10-C8-C7
31	d	402	CLA	C6-C7-C8-C10
31	n	603	CLA	C12-C13-C15-C16
31	y	611	CLA	C12-C13-C15-C16
31	B1	602	CLA	C12-C13-C15-C16
31	B1	613	CLA	C11-C10-C8-C7
31	C1	501	CLA	C11-C12-C13-C15
31	C1	507	CLA	C6-C7-C8-C10
31	C1	511	CLA	C11-C12-C13-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C1	512	CLA	C11-C10-C8-C7
31	N1	613	CLA	C11-C12-C13-C15
31	N1	613	CLA	C12-C13-C15-C16
31	G1	602	CLA	C12-C13-C15-C16
31	R1	612	CLA	C6-C7-C8-C10
31	Y1	604	CLA	C6-C7-C8-C10
31	Y1	614	CLA	C11-C10-C8-C7
31	b1	602	CLA	C11-C10-C8-C7
31	b1	613	CLA	C11-C10-C8-C7
31	c1	513	CLA	C11-C10-C8-C7
31	d1	402	CLA	C6-C7-C8-C10
31	g1	602	CLA	C12-C13-C15-C16
31	g1	610	CLA	C12-C13-C15-C16
31	s1	610	CLA	C6-C7-C8-C10
31	s1	611	CLA	C11-C12-C13-C15
31	y1	604	CLA	C6-C7-C8-C10
31	y1	613	CLA	C12-C13-C15-C16
32	a	409	PHO	C6-C7-C8-C10
32	A1	409	PHO	C6-C7-C8-C10
32	a1	409	PHO	C6-C7-C8-C10
41	d	410	LHG	O6-C4-C5-O7
41	g	624	LHG	O6-C4-C5-O7
41	G1	624	LHG	O6-C4-C5-O7
41	c1	525	LHG	O6-C4-C5-O7
47	N	606	CHL	C11-C12-C13-C15
47	N	609	CHL	C11-C10-C8-C7
47	n	606	CHL	C11-C10-C8-C7
47	n	609	CHL	C11-C10-C8-C7
47	g	609	CHL	C11-C10-C8-C7
47	G1	601	CHL	C6-C7-C8-C10
47	G1	607	CHL	C11-C12-C13-C15
47	n1	601	CHL	C11-C12-C13-C15
47	g1	609	CHL	C11-C12-C13-C15
48	R	620	LUT	C25-C26-C27-C28
48	S	621	LUT	C25-C26-C27-C28
48	s	620	LUT	C25-C26-C27-C28
48	R1	620	LUT	C25-C26-C27-C28
48	S1	621	LUT	C25-C26-C27-C28
48	r1	620	LUT	C25-C26-C27-C28
48	s1	621	LUT	C25-C26-C27-C28
52	B1	624	3PH	O11-C1-C2-O21
57	Y1	627	PTY	O14-C5-C6-O7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	c	626	SQD	C9-C10-C11-C12
31	c	511	CLA	C10-C11-C12-C13
38	c	524	DGA	CA8-CA9-CAA-CBA
40	C	518	DGD	C2B-C3B-C4B-C5B
41	D1	410	LHG	C10-C11-C12-C13
33	a1	411	BCR	C9-C10-C11-C12
38	B	625	DGA	CBB-CAB-CB9-CB8
38	J1	101	DGA	CB6-CB7-CB8-CB9
31	C1	511	CLA	C8-C10-C11-C12
31	Y1	603	CLA	C15-C16-C17-C18
35	b1	622	LMG	C4-C5-C6-O5
41	c1	525	LHG	C8-C7-O7-C5
41	y1	624	LHG	C8-C7-O7-C5
41	D	408	LHG	C31-C32-C33-C34
41	d	409	LHG	C31-C32-C33-C34
41	s	624	LHG	C34-C35-C36-C37
41	d1	408	LHG	C34-C35-C36-C37
40	B1	623	DGD	O1A-C1A-O1G-C1G
52	T1	101	3PH	C3A-C3B-C3C-C3D
53	A1	414	SPH	C13-C14-C15-C16
31	n	613	CLA	C10-C11-C12-C13
31	r	609	CLA	C10-C11-C12-C13
31	a	405	CLA	C2A-CAA-CBA-CGA
31	c	506	CLA	C2A-CAA-CBA-CGA
31	G1	610	CLA	C2A-CAA-CBA-CGA
34	B1	626	SQD	C10-C11-C12-C13
31	R	603	CLA	C3-C5-C6-C7
35	H1	102	LMG	C10-C11-C12-C13
34	B	621	SQD	C44-C45-C46-O48
34	b	621	SQD	C44-C45-C46-O48
34	M1	101	SQD	C26-C27-C28-C29
34	c1	526	SQD	O6-C44-C45-C46
35	J	101	LMG	C7-C8-C9-O8
35	j	101	LMG	C7-C8-C9-O8
35	B1	622	LMG	O1-C7-C8-C9
35	C1	521	LMG	C7-C8-C9-O8
35	w1	201	LMG	C7-C8-C9-O8
40	C	523	DGD	O1G-C1G-C2G-C3G
41	N	624	LHG	C24-C25-C26-C27
41	N1	624	LHG	C4-C5-C6-O8
41	c1	525	LHG	C4-C5-C6-O8
41	g1	624	LHG	C4-C5-C6-O8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
52	T1	101	3PH	C32-C33-C34-C35
53	y	625	SPH	O1-C1-C2-N2
54	k1	101	4RF	C28-C29-C30-C31
31	y	613	CLA	O1A-CGA-O2A-C1
34	A1	412	SQD	O6-C44-C45-O47
34	m1	101	SQD	O47-C45-C46-O48
35	c	521	LMG	O1-C7-C8-O7
35	B1	622	LMG	O7-C8-C9-O8
35	C1	523	LMG	O1-C7-C8-O7
35	a1	413	LMG	O7-C8-C9-O8
40	c	523	DGD	O1G-C1G-C2G-O2G
40	b1	623	DGD	O1G-C1G-C2G-O2G
40	c1	520	DGD	O1G-C1G-C2G-O2G
41	L	101	LHG	O7-C5-C6-O8
41	c	625	LHG	O7-C5-C6-O8
41	d	408	LHG	O7-C5-C6-O8
41	l	101	LHG	O7-C5-C6-O8
41	s	624	LHG	O7-C5-C6-O8
41	d1	409	LHG	O7-C5-C6-O8
42	c	627	LMK	O1-C7-C8-O7
42	C1	527	LMK	O1-C7-C8-O7
54	K1	101	4RF	O18-C19-C20-O21
54	k1	101	4RF	O18-C19-C20-O21
57	y1	626	PTY	O4-C1-C6-O7
41	d	410	LHG	C33-C34-C35-C36
41	s	624	LHG	C11-C10-C9-C8
34	b	621	SQD	C27-C28-C29-C30
41	y	624	LHG	C15-C16-C17-C18
40	c	518	DGD	C5A-C6A-C7A-C8A
34	A	412	SQD	C45-C44-O6-C1
34	a	412	SQD	C45-C44-O6-C1
35	J	101	LMG	C8-C7-O1-C1
35	W1	201	LMG	C8-C7-O1-C1
40	C1	519	DGD	C5D-C6D-O5D-C1E
35	h1	102	LMG	O7-C10-C11-C12
31	Y	611	CLA	C16-C17-C18-C19
31	B1	615	CLA	C16-C17-C18-C19
31	b1	614	CLA	C13-C15-C16-C17
41	D1	409	LHG	C24-C25-C26-C27
32	A1	409	PHO	O1D-CGD-O2D-CED
34	B1	626	SQD	C29-C30-C31-C32
34	b1	626	SQD	C19-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
40	C	523	DGD	C9B-CAB-CBB-CCB
52	s1	626	3PH	C2C-C2D-C2E-C2F
38	C	524	DGA	OA1-CA1-OG1-CG1
31	c	510	CLA	C15-C16-C17-C18
31	A1	410	CLA	C10-C11-C12-C13
31	n	602	CLA	C4-C3-C5-C6
47	n	609	CHL	C4-C3-C5-C6
31	B	607	CLA	CBA-CGA-O2A-C1
31	y	613	CLA	CBA-CGA-O2A-C1
31	d1	402	CLA	CBA-CGA-O2A-C1
34	B1	621	SQD	C9-C10-C11-C12
35	A1	413	LMG	C36-C37-C38-C39
31	C	506	CLA	C2-C3-C5-C6
31	G	602	CLA	C2-C3-C5-C6
31	r	609	CLA	C2-C3-C5-C6
31	y1	611	CLA	C2-C3-C5-C6
41	D	408	LHG	C9-C10-C11-C12
41	N	624	LHG	C28-C29-C30-C31
41	n1	624	LHG	C29-C30-C31-C32
51	S	625	LPX	C11-C10-C9-C8
31	d	403	CLA	C13-C15-C16-C17
31	n	603	CLA	C8-C10-C11-C12
31	A	406	CLA	C11-C10-C8-C9
31	C	502	CLA	C11-C12-C13-C14
31	C	503	CLA	C11-C10-C8-C9
31	C	505	CLA	C14-C13-C15-C16
31	C	510	CLA	C6-C7-C8-C9
31	N	602	CLA	C11-C10-C8-C9
31	G	613	CLA	C14-C13-C15-C16
31	S	603	CLA	C11-C10-C8-C9
31	Y	602	CLA	C11-C10-C8-C9
31	Y	603	CLA	C6-C7-C8-C9
31	b	612	CLA	C6-C7-C8-C9
31	b	615	CLA	C11-C12-C13-C14
31	c	508	CLA	C14-C13-C15-C16
31	c	512	CLA	C11-C10-C8-C9
31	n	610	CLA	C6-C7-C8-C9
31	n	613	CLA	C14-C13-C15-C16
31	s	603	CLA	C11-C12-C13-C14
31	y	612	CLA	C11-C12-C13-C14
31	y	614	CLA	C11-C10-C8-C9
31	B1	603	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B1	608	CLA	C14-C13-C15-C16
31	B1	616	CLA	C11-C12-C13-C14
31	D1	403	CLA	C6-C7-C8-C9
31	S1	610	CLA	C11-C12-C13-C14
31	S1	611	CLA	C11-C12-C13-C14
31	Y1	610	CLA	C11-C12-C13-C14
31	Y1	612	CLA	C11-C10-C8-C9
31	Y1	614	CLA	C11-C10-C8-C9
31	b1	602	CLA	C11-C10-C8-C9
31	b1	615	CLA	C6-C7-C8-C9
31	c1	507	CLA	C11-C10-C8-C9
31	n1	602	CLA	C11-C10-C8-C9
31	n1	613	CLA	C11-C10-C8-C9
31	g1	602	CLA	C6-C7-C8-C9
31	g1	602	CLA	C14-C13-C15-C16
31	r1	603	CLA	C11-C10-C8-C9
31	y1	602	CLA	C14-C13-C15-C16
31	y1	604	CLA	C14-C13-C15-C16
31	y1	614	CLA	C11-C12-C13-C14
32	a	409	PHO	C11-C10-C8-C9
47	N	606	CHL	C11-C10-C8-C9
47	g	609	CHL	C11-C12-C13-C14
47	N1	601	CHL	C14-C13-C15-C16
47	N1	606	CHL	C11-C12-C13-C14
47	Y1	607	CHL	C11-C10-C8-C9
47	n1	601	CHL	C14-C13-C15-C16
47	y1	606	CHL	C11-C10-C8-C9
41	y1	624	LHG	O9-C7-O7-C5
41	C	525	LHG	C14-C15-C16-C17
41	D	410	LHG	C33-C34-C35-C36
52	i	101	3PH	C22-C23-C24-C25
42	c1	527	LMK	O7-C10-C11-C12
47	N1	606	CHL	C3-C5-C6-C7
44	D	405	PL9	C29-C31-C32-C33
34	B1	621	SQD	C28-C29-C30-C31
54	K1	101	4RF	C11-C12-C13-C14
34	B1	626	SQD	C7-C8-C9-C10
31	B	607	CLA	O1A-CGA-O2A-C1
31	A1	410	CLA	O1A-CGA-O2A-C1
31	d1	402	CLA	O1A-CGA-O2A-C1
31	A1	410	CLA	C2A-CAA-CBA-CGA
31	C1	501	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	d	402	CLA	CAA-CBA-CGA-O2A
41	C	525	LHG	O1-C1-C2-O2
42	c1	527	LMK	O9-C10-C11-C12
35	J	101	LMG	C16-C17-C18-C19
33	D	404	BCR	C18-C19-C20-C21
33	d	404	BCR	C18-C19-C20-C21
33	D1	404	BCR	C13-C14-C15-C16
48	r1	620	LUT	C29-C30-C31-C32
49	r	622	XAT	C33-C34-C35-C15
41	L1	101	LHG	C34-C35-C36-C37
31	B1	604	CLA	C13-C15-C16-C17
47	g1	601	CHL	C5-C6-C7-C8
35	h	102	LMG	C15-C16-C17-C18
40	C	523	DGD	C1A-C2A-C3A-C4A
31	a1	410	CLA	C11-C12-C13-C15
41	D	408	LHG	C34-C35-C36-C37
41	c	625	LHG	C10-C11-C12-C13
51	s	625	LPX	C11-C10-C9-C8
54	K1	101	4RF	C33-C34-C35-C36
33	C1	515	BCR	C17-C18-C19-C20
31	r	609	CLA	CAA-CBA-CGA-O2A
38	c	524	DGA	CB3-CB4-CB5-CB6
31	c1	513	CLA	O1A-CGA-O2A-C1
35	b1	622	LMG	C21-C22-C23-C24
41	Y	624	LHG	C24-C25-C26-C27
31	c	513	CLA	C15-C16-C17-C18
50	s	623	NEX	C39-C29-C30-C31
50	Y1	623	NEX	C39-C29-C30-C31
52	b1	624	3PH	C33-C34-C35-C36
52	b1	624	3PH	C39-C3A-C3B-C3C
31	s	604	CLA	C4-C3-C5-C6
31	C1	505	CLA	CBD-CGD-O2D-CED
34	C	526	SQD	C12-C13-C14-C15
40	C	520	DGD	C5A-C6A-C7A-C8A
40	c	523	DGD	C3A-C4A-C5A-C6A
41	Y	624	LHG	C27-C28-C29-C30
41	L1	101	LHG	C33-C34-C35-C36
54	I1	102	4RF	C52-C53-C54-C55
57	y1	626	PTY	C17-C18-C19-C20
31	R	602	CLA	C2-C3-C5-C6
31	r	603	CLA	C2-C3-C5-C6
31	C1	509	CLA	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	N	609	CHL	C2-C3-C5-C6
31	s	602	CLA	C5-C6-C7-C8
52	T1	101	3PH	C25-C26-C27-C28
44	D	405	PL9	C47-C48-C49-C51
41	D	409	LHG	C19-C20-C21-C22
31	R1	610	CLA	C8-C10-C11-C12
31	N	611	CLA	C1-C2-C3-C4
31	G	604	CLA	C1-C2-C3-C4
31	G	614	CLA	C1-C2-C3-C4
31	n	611	CLA	C1-C2-C3-C4
31	g	604	CLA	C1-C2-C3-C4
31	g	614	CLA	C1-C2-C3-C4
31	N1	611	CLA	C1-C2-C3-C4
31	G1	604	CLA	C1-C2-C3-C4
31	G1	614	CLA	C1-C2-C3-C4
31	n1	611	CLA	C1-C2-C3-C4
31	g1	604	CLA	C1-C2-C3-C4
31	g1	614	CLA	C1-C2-C3-C4
47	N	608	CHL	C1-C2-C3-C4
47	G	606	CHL	C1-C2-C3-C4
47	G	607	CHL	C1-C2-C3-C4
47	n	608	CHL	C1-C2-C3-C4
47	g	606	CHL	C1-C2-C3-C4
47	g	607	CHL	C1-C2-C3-C4
47	r	607	CHL	C1-C2-C3-C4
47	N1	608	CHL	C1-C2-C3-C4
47	G1	606	CHL	C1-C2-C3-C4
47	R1	607	CHL	C1-C2-C3-C4
47	n1	608	CHL	C1-C2-C3-C4
47	g1	606	CHL	C1-C2-C3-C4
47	r1	607	CHL	C1-C2-C3-C4
40	c1	518	DGD	C4D-C5D-C6D-O5D
34	A1	412	SQD	O10-C23-O48-C46
35	H	102	LMG	C15-C16-C17-C18
35	d1	411	LMG	C18-C19-C20-C21
52	B1	624	3PH	C39-C3A-C3B-C3C
31	c1	510	CLA	C3-C5-C6-C7
31	N	613	CLA	CAA-CBA-CGA-O2A
42	c1	527	LMK	C13-C14-C15-C27
31	C1	508	CLA	C5-C6-C7-C8
31	c1	508	CLA	C8-C10-C11-C12
35	B1	622	LMG	C9-C8-O7-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	b1	622	LMG	C9-C8-O7-C10
38	b1	625	DGA	CG1-CG2-OG2-CB1
40	B1	623	DGD	C3G-C2G-O2G-C1B
41	N	624	LHG	C6-C5-O7-C7
52	S1	626	3PH	C1-C2-O21-C21
57	y1	626	PTY	O14-C5-C6-C1
31	B	607	CLA	C2A-CAA-CBA-CGA
31	g	602	CLA	C2A-CAA-CBA-CGA
31	S1	609	CLA	C2A-CAA-CBA-CGA
31	s1	613	CLA	C2A-CAA-CBA-CGA
34	M1	101	SQD	C25-C26-C27-C28
41	L	101	LHG	C19-C20-C21-C22
41	Y1	624	LHG	C32-C33-C34-C35
35	h1	102	LMG	O9-C10-O7-C8
31	c1	513	CLA	CBA-CGA-O2A-C1
31	S	604	CLA	C2-C1-O2A-CGA
31	Y	604	CLA	C2-C1-O2A-CGA
31	c	512	CLA	C2-C1-O2A-CGA
31	B1	607	CLA	C2-C1-O2A-CGA
31	B1	612	CLA	C2-C1-O2A-CGA
31	Y1	610	CLA	C2-C1-O2A-CGA
31	b1	602	CLA	C2-C1-O2A-CGA
31	c1	505	CLA	C2-C1-O2A-CGA
31	s1	604	CLA	C2-C1-O2A-CGA
31	s1	609	CLA	C2-C1-O2A-CGA
31	y1	613	CLA	C2-C1-O2A-CGA
47	G	609	CHL	C2-C1-O2A-CGA
47	Y	606	CHL	C2-C1-O2A-CGA
47	g	601	CHL	C2-C1-O2A-CGA
47	r	607	CHL	C2-C1-O2A-CGA
47	g1	601	CHL	C2-C1-O2A-CGA
31	N	604	CLA	C16-C17-C18-C20
31	Y1	610	CLA	C16-C17-C18-C19
38	C1	524	DGA	CA3-CA4-CA5-CA6
32	A1	409	PHO	CBD-CGD-O2D-CED
31	N1	613	CLA	CAA-CBA-CGA-O2A
47	S1	608	CHL	CAA-CBA-CGA-O2A
54	I1	102	4RF	C14-C15-C16-O18
31	b	603	CLA	C5-C6-C7-C8
31	D1	402	CLA	C3-C5-C6-C7
38	c1	524	DGA	CFA-CGA-CHA-CIA
41	c	625	LHG	C25-C26-C27-C28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	d	409	LHG	C35-C36-C37-C38
41	l	101	LHG	C2-C3-O3-P
41	D1	409	LHG	C2-C3-O3-P
51	S	625	LPX	C4-C3-O1-P1
50	g	623	NEX	C13-C14-C15-C35
41	l	101	LHG	O6-C4-C5-O7
41	D1	409	LHG	O6-C4-C5-O7
41	N1	624	LHG	O6-C4-C5-O7
38	c1	524	DGA	CA2-CA3-CA4-CA5
41	Y	624	LHG	C29-C30-C31-C32
41	s	624	LHG	C10-C11-C12-C13
31	C1	509	CLA	C16-C17-C18-C19
31	A	405	CLA	C10-C11-C12-C13
31	N	610	CLA	C8-C10-C11-C12
31	b	612	CLA	C5-C6-C7-C8
31	g1	602	CLA	C15-C16-C17-C18
35	d1	411	LMG	C10-C11-C12-C13
31	c	506	CLA	C4-C3-C5-C6
44	D1	405	PL9	C40-C39-C41-C42
41	N1	624	LHG	C14-C15-C16-C17
33	c	515	BCR	C23-C24-C25-C26
33	c	515	BCR	C23-C24-C25-C30
33	c	517	BCR	C5-C6-C7-C8
33	C1	515	BCR	C23-C24-C25-C26
33	c1	515	BCR	C5-C6-C7-C8
37	B	620	C7Z	C21-C26-C27-C28
48	r	620	LUT	C1-C6-C7-C8
48	y1	621	LUT	C1-C6-C7-C8
31	c1	508	CLA	C2-C3-C5-C6
41	d1	409	LHG	C35-C36-C37-C38
31	Y	608	CLA	CBA-CGA-O2A-C1
31	B1	610	CLA	C8-C10-C11-C12
31	Y	603	CLA	C16-C17-C18-C20
31	B1	605	CLA	C16-C17-C18-C20
31	n1	613	CLA	C16-C17-C18-C20
47	n	607	CHL	C16-C17-C18-C20
35	h1	102	LMG	C11-C10-O7-C8
38	C1	524	DGA	CB2-CB1-OG2-CG2
35	w1	201	LMG	O6-C1-O1-C7
40	c1	518	DGD	O6E-C1E-O5D-C6D
34	C1	526	SQD	C27-C28-C29-C30
31	Y	604	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	b	610	CLA	C13-C15-C16-C17
31	Y1	603	CLA	C10-C11-C12-C13
31	C	502	CLA	C2A-CAA-CBA-CGA
47	y1	606	CHL	C2A-CAA-CBA-CGA
40	c1	518	DGD	C2E-C1E-O5D-C6D
50	S	622	NEX	C28-C29-C30-C31
50	s	623	NEX	C28-C29-C30-C31
50	Y1	623	NEX	C28-C29-C30-C31
50	n1	623	NEX	C28-C29-C30-C31
34	c	626	SQD	O47-C45-C46-O48
41	D1	409	LHG	O7-C5-C6-O8
31	B	606	CLA	C10-C11-C12-C13
31	Y	612	CLA	C13-C15-C16-C17
35	H1	102	LMG	C11-C12-C13-C14
51	s1	625	LPX	C7-C8-C9-C10
31	b1	615	CLA	CBA-CGA-O2A-C1
41	D	409	LHG	C4-O6-P-O3
41	L	101	LHG	C4-O6-P-O3
41	N	624	LHG	C3-O3-P-O6
41	G	630	LHG	C3-O3-P-O6
41	Y	624	LHG	C3-O3-P-O6
41	d	408	LHG	C3-O3-P-O6
41	d	409	LHG	C3-O3-P-O6
41	d	409	LHG	C4-O6-P-O3
41	n	624	LHG	C3-O3-P-O6
41	g	624	LHG	C3-O3-P-O6
41	s	624	LHG	C3-O3-P-O6
41	D1	409	LHG	C4-O6-P-O3
41	L1	101	LHG	C4-O6-P-O3
41	N1	624	LHG	C3-O3-P-O6
41	G1	624	LHG	C3-O3-P-O6
41	S1	624	LHG	C3-O3-P-O6
41	Y1	624	LHG	C3-O3-P-O6
41	d1	408	LHG	C4-O6-P-O3
41	n1	624	LHG	C3-O3-P-O6
41	g1	624	LHG	C3-O3-P-O6
41	y1	624	LHG	C3-O3-P-O6
51	S	625	LPX	C3-O1-P1-O2
35	h	102	LMG	C16-C17-C18-C19
38	c1	524	DGA	CB3-CB4-CB5-CB6
47	N	607	CHL	C8-C10-C11-C12
41	y	624	LHG	C34-C35-C36-C37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
52	T1	101	3PH	C37-C38-C39-C3A
47	n	607	CHL	C16-C17-C18-C19
32	A	409	PHO	CHA-CBD-CGD-O1D
32	A	409	PHO	CHA-CBD-CGD-O2D
32	a	409	PHO	CHA-CBD-CGD-O2D
32	A1	408	PHO	CHA-CBD-CGD-O1D
32	A1	408	PHO	CHA-CBD-CGD-O2D
34	a1	412	SQD	C25-C26-C27-C28
34	B1	626	SQD	C14-C15-C16-C17
34	a1	412	SQD	O6-C44-C45-C46
35	a	413	LMG	C7-C8-C9-O8
35	D1	411	LMG	C7-C8-C9-O8
38	b	623	DGA	OG1-CG1-CG2-CG3
41	Y1	624	LHG	C4-C5-C6-O8
54	K1	101	4RF	O18-C19-C20-C39
31	B	617	CLA	C4-C3-C5-C6
44	D	405	PL9	C35-C34-C36-C37
34	a1	412	SQD	C9-C10-C11-C12
41	g1	624	LHG	C25-C26-C27-C28
54	k1	101	4RF	C02-C03-C04-C05
31	B	612	CLA	C11-C12-C13-C15
31	B	617	CLA	C11-C12-C13-C15
31	b	604	CLA	C11-C12-C13-C15
31	g	602	CLA	C11-C10-C8-C7
31	s	603	CLA	C11-C12-C13-C15
31	b1	604	CLA	C6-C7-C8-C10
31	n1	602	CLA	C11-C12-C13-C15
31	r1	602	CLA	C11-C10-C8-C7
31	r1	603	CLA	C11-C10-C8-C7
31	y1	603	CLA	C6-C7-C8-C10
47	n1	606	CHL	C11-C10-C8-C7
34	C1	526	SQD	C17-C18-C19-C20
34	C1	526	SQD	C30-C31-C32-C33
41	Y	624	LHG	C16-C17-C18-C19
52	T1	101	3PH	C2D-C2E-C2F-C2G
31	R	608	CLA	C6-C7-C8-C9
31	a	405	CLA	C6-C7-C8-C9
31	b	605	CLA	C11-C10-C8-C9
31	b	613	CLA	C11-C10-C8-C9
31	n	603	CLA	C14-C13-C15-C16
31	s	602	CLA	C11-C10-C8-C9
31	s	609	CLA	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	y	611	CLA	C14-C13-C15-C16
31	B1	613	CLA	C11-C10-C8-C9
31	C1	501	CLA	C11-C12-C13-C14
31	C1	505	CLA	C11-C12-C13-C14
31	C1	506	CLA	C14-C13-C15-C16
31	C1	507	CLA	C6-C7-C8-C9
31	C1	507	CLA	C14-C13-C15-C16
31	N1	610	CLA	C14-C13-C15-C16
31	R1	610	CLA	C11-C10-C8-C9
31	Y1	603	CLA	C14-C13-C15-C16
31	b1	610	CLA	C6-C7-C8-C9
31	b1	613	CLA	C11-C10-C8-C9
31	g1	603	CLA	C14-C13-C15-C16
31	s1	611	CLA	C14-C13-C15-C16
31	y1	613	CLA	C14-C13-C15-C16
32	A1	409	PHO	C6-C7-C8-C9
47	N	605	CHL	C14-C13-C15-C16
47	N	609	CHL	C11-C10-C8-C9
47	n	606	CHL	C11-C10-C8-C9
47	n	609	CHL	C11-C10-C8-C9
47	N1	605	CHL	C11-C12-C13-C14
47	G1	609	CHL	C11-C12-C13-C14
41	d	409	LHG	C8-C7-O7-C5
33	D	404	BCR	C9-C10-C11-C12
33	a	411	BCR	C9-C10-C11-C12
33	a	411	BCR	C13-C14-C15-C16
33	a	411	BCR	C15-C16-C17-C18
33	c1	515	BCR	C19-C20-C21-C22
37	B1	620	C7Z	C13-C14-C15-C35
48	S	620	LUT	C29-C30-C31-C32
48	Y	620	LUT	C29-C30-C31-C32
48	G1	620	LUT	C33-C34-C35-C15
48	S1	621	LUT	C29-C30-C31-C32
48	s1	620	LUT	C29-C30-C31-C32
50	G	623	NEX	C9-C10-C11-C12
31	b1	617	CLA	C16-C17-C18-C19
41	g	624	LHG	C12-C13-C14-C15
38	C1	524	DGA	OB1-CB1-OG2-CG2
35	B	622	LMG	C21-C22-C23-C24
31	A1	410	CLA	CBA-CGA-O2A-C1
31	B	612	CLA	C13-C15-C16-C17
31	Y	608	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	b1	626	SQD	C13-C14-C15-C16
38	B1	625	DGA	CFB-CGB-CHB-CIB
31	S1	613	CLA	C5-C6-C7-C8
52	b1	624	3PH	C27-C28-C29-C2A
31	r1	603	CLA	C3-C5-C6-C7
52	t1	101	3PH	C32-C33-C34-C35
37	B	620	C7Z	C11-C12-C13-C20
48	g	620	LUT	C27-C28-C29-C39
49	R	621	XAT	C31-C32-C33-C40
31	B	612	CLA	C5-C6-C7-C8
31	b	615	CLA	C16-C17-C18-C20
54	I1	102	4RF	C47-C48-C49-C50
41	D	410	LHG	C5-C4-O6-P
41	D1	408	LHG	C2-C3-O3-P
34	b1	626	SQD	C10-C11-C12-C13
40	C	519	DGD	C5B-C6B-C7B-C8B
41	c	625	LHG	C16-C17-C18-C19
31	b	612	CLA	C13-C15-C16-C17
31	A1	405	CLA	C15-C16-C17-C18
31	b1	605	CLA	C13-C15-C16-C17
31	y1	602	CLA	C8-C10-C11-C12
33	C	515	BCR	C21-C22-C23-C24
33	c	514	BCR	C21-C22-C23-C24
37	B1	620	C7Z	C11-C12-C13-C14
41	n	624	LHG	C11-C10-C9-C8
41	S1	624	LHG	C24-C25-C26-C27
42	c1	527	LMK	C28-C29-C30-C31
34	b1	621	SQD	C12-C13-C14-C15
35	d	411	LMG	C11-C12-C13-C14
40	C	518	DGD	C6A-C7A-C8A-C9A
41	L	101	LHG	O9-C7-O7-C5
41	d1	408	LHG	O9-C7-O7-C5
52	s	626	3PH	C2C-C2D-C2E-C2F
31	s1	610	CLA	C4-C3-C5-C6
44	d	405	PL9	C20-C19-C21-C22
52	B1	624	3PH	C21-C22-C23-C24
52	b1	624	3PH	C21-C22-C23-C24
44	D	405	PL9	C28-C29-C31-C32
47	G1	609	CHL	C2-C3-C5-C6
31	B	609	CLA	C16-C17-C18-C20
31	c	505	CLA	C16-C17-C18-C19
31	s	610	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	D1	402	CLA	CBA-CGA-O2A-C1
35	h	102	LMG	C19-C20-C21-C22
51	S1	625	LPX	C11-C12-C13-C14
51	s1	625	LPX	C12-C13-C14-C15
41	d1	409	LHG	O10-C23-O8-C6
41	D1	409	LHG	C32-C33-C34-C35
41	L1	101	LHG	C17-C18-C19-C20
31	B	609	CLA	C13-C15-C16-C17
31	b1	607	CLA	C15-C16-C17-C18
41	c1	525	LHG	C24-C25-C26-C27
54	K1	101	4RF	C09-C10-C11-C12
47	N	607	CHL	CAA-CBA-CGA-O2A
34	C1	526	SQD	C28-C29-C30-C31
41	C	525	LHG	C33-C34-C35-C36
41	N1	624	LHG	C30-C31-C32-C33
31	R	609	CLA	C10-C11-C12-C13
31	b1	615	CLA	O1A-CGA-O2A-C1
31	b	610	CLA	CBA-CGA-O2A-C1
53	y	625	SPH	C14-C15-C16-C17
47	N	607	CHL	C2A-CAA-CBA-CGA
31	B	605	CLA	C16-C17-C18-C20
41	g	624	LHG	O10-C23-C24-C25
33	A	411	BCR	C19-C20-C21-C22
33	c	516	BCR	C13-C14-C15-C16
33	B1	619	BCR	C13-C14-C15-C16
33	C1	514	BCR	C19-C20-C21-C22
33	c1	514	BCR	C13-C14-C15-C16
37	B1	620	C7Z	C33-C34-C35-C15
37	B1	620	C7Z	C29-C30-C31-C32
48	N	620	LUT	C9-C10-C11-C12
48	G	621	LUT	C29-C30-C31-C32
48	g	620	LUT	C29-C30-C31-C32
48	G1	621	LUT	C9-C10-C11-C12
48	Y1	620	LUT	C29-C30-C31-C32
48	y1	621	LUT	C33-C34-C35-C15
50	y	623	NEX	C29-C30-C31-C32
50	y1	623	NEX	C29-C30-C31-C32
35	H1	102	LMG	C12-C13-C14-C15
41	d	409	LHG	O9-C7-O7-C5
57	y1	626	PTY	N1-C2-C3-O11
31	c1	504	CLA	C15-C16-C17-C18
31	g1	610	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
35	d1	411	LMG	C21-C22-C23-C24
54	I1	102	4RF	C24-C25-C26-C27
52	s1	626	3PH	O11-C1-C2-O21
47	r1	607	CHL	C2C-C3C-CAC-CBC
51	S1	625	LPX	C12-C13-C14-C15
33	C1	517	BCR	C10-C11-C12-C13
33	c1	516	BCR	C10-C11-C12-C13
50	n	623	NEX	C30-C31-C32-C33
31	y	602	CLA	C16-C17-C18-C19
31	b1	608	CLA	C16-C17-C18-C20
47	N	605	CHL	C3-C5-C6-C7
57	Y1	626	PTY	C31-C32-C33-C34
31	g	610	CLA	C4-C3-C5-C6
47	y	606	CHL	C4-C3-C5-C6
31	C	509	CLA	C5-C6-C7-C8
31	y	610	CLA	C5-C6-C7-C8
31	S1	610	CLA	C8-C10-C11-C12
52	s	626	3PH	C33-C34-C35-C36
31	B	609	CLA	C2-C3-C5-C6
31	D1	402	CLA	O1A-CGA-O2A-C1
35	c1	523	LMG	C13-C14-C15-C16
40	C	518	DGD	CAB-CBB-CCB-CDB
41	d	409	LHG	C30-C31-C32-C33
41	N1	624	LHG	C29-C30-C31-C32
52	T1	101	3PH	C2A-C2B-C2C-C2D
53	A1	414	SPH	C7-C8-C9-C10
42	c1	527	LMK	C2-C3-C4-O2
31	g1	614	CLA	C2-C1-O2A-CGA
32	A	409	PHO	C2-C1-O2A-CGA
47	n	607	CHL	C2-C1-O2A-CGA
31	c	506	CLA	C15-C16-C17-C18
31	y	610	CLA	C15-C16-C17-C18
51	S1	625	LPX	C6-C7-C8-C9
34	B1	621	SQD	C13-C14-C15-C16
41	l	101	LHG	C12-C13-C14-C15
56	R1	626	ERG	C22-C23-C24-C28
52	i	101	3PH	C3C-C3D-C3E-C3F
31	A	406	CLA	C2A-CAA-CBA-CGA
31	N1	612	CLA	C2A-CAA-CBA-CGA
31	S1	611	CLA	C2A-CAA-CBA-CGA
31	s1	611	CLA	C2A-CAA-CBA-CGA
31	c	504	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	b1	621	SQD	C14-C15-C16-C17
52	B1	624	3PH	C2-C1-O11-P
31	C	506	CLA	C3A-C2A-CAA-CBA
31	C	512	CLA	C3A-C2A-CAA-CBA
31	b	612	CLA	C3A-C2A-CAA-CBA
31	b	613	CLA	C3A-C2A-CAA-CBA
31	y1	613	CLA	C3A-C2A-CAA-CBA
47	S	608	CHL	C3A-C2A-CAA-CBA
47	Y	609	CHL	C3A-C2A-CAA-CBA
47	n	608	CHL	C3A-C2A-CAA-CBA
47	y	601	CHL	C3A-C2A-CAA-CBA
31	c1	512	CLA	C16-C17-C18-C19
34	c1	526	SQD	C25-C26-C27-C28
41	D	410	LHG	C26-C27-C28-C29
41	N1	624	LHG	C19-C20-C21-C22
41	l	101	LHG	O9-C7-O7-C5
47	N	608	CHL	O2A-C1-C2-C3
47	n1	608	CHL	O2A-C1-C2-C3
47	g1	607	CHL	CAA-CBA-CGA-O2A
35	b	622	LMG	C11-C12-C13-C14
41	Y	624	LHG	C19-C20-C21-C22
41	D1	410	LHG	C25-C26-C27-C28
48	g	620	LUT	C33-C34-C35-C15
50	G	623	NEX	C13-C14-C15-C35
38	b	623	DGA	CFA-CGA-CHA-CIA
38	c1	524	DGA	CB5-CB6-CB7-CB8
41	D1	410	LHG	C9-C10-C11-C12
53	y	625	SPH	C9-C10-C11-C12
31	b	610	CLA	C4-C3-C5-C6
31	C1	506	CLA	C4-C3-C5-C6
31	n1	613	CLA	C4-C3-C5-C6
47	N1	609	CHL	C4-C3-C5-C6
34	B1	626	SQD	C32-C33-C34-C35
41	n1	624	LHG	C16-C17-C18-C19
53	Y1	625	SPH	C13-C14-C15-C16
35	b	622	LMG	C18-C19-C20-C21
38	c1	524	DGA	CAA-CBA-CCA-CDA
40	C1	519	DGD	C3A-C4A-C5A-C6A
31	G	602	CLA	C11-C10-C8-C9
31	b	603	CLA	C11-C10-C8-C9
31	c	508	CLA	C11-C10-C8-C9
31	B1	604	CLA	C14-C13-C15-C16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	C1	511	CLA	C14-C13-C15-C16
31	a1	406	CLA	C6-C7-C8-C9
31	b1	602	CLA	C11-C12-C13-C14
31	b1	617	CLA	C11-C10-C8-C9
31	c1	510	CLA	C11-C12-C13-C14
31	g1	602	CLA	C11-C10-C8-C9
31	g1	611	CLA	C11-C12-C13-C14
32	A	408	PHO	C11-C10-C8-C9
47	n	607	CHL	C14-C13-C15-C16
47	G1	609	CHL	C11-C10-C8-C9
51	s	625	LPX	C16-C17-C18-C19
52	S	626	3PH	C38-C39-C3A-C3B
54	I1	102	4RF	C04-C05-C06-C07
31	Y	603	CLA	C10-C11-C12-C13
31	D1	402	CLA	C5-C6-C7-C8
35	h1	102	LMG	C12-C13-C14-C15
38	b	623	DGA	CBB-CCB-CDB-CEB
47	G	609	CHL	C4C-C3C-CAC-CBC
34	a	412	SQD	C35-C36-C37-C38
41	d	408	LHG	C31-C32-C33-C34
41	d	409	LHG	C27-C28-C29-C30
33	D	404	BCR	C20-C21-C22-C37
33	d	404	BCR	C20-C21-C22-C37
34	c	626	SQD	C44-C45-C46-O48
40	C	519	DGD	O1G-C1G-C2G-C3G
48	G	621	LUT	C21-C26-C27-C28
50	N	623	NEX	C39-C29-C30-C31
50	G1	623	NEX	C39-C29-C30-C31
50	S1	623	NEX	C39-C29-C30-C31
50	Y1	623	NEX	C40-C33-C34-C35
50	n1	623	NEX	C39-C29-C30-C31
38	C	524	DGA	CDA-CEA-CFA-CGA
31	c	502	CLA	C2A-CAA-CBA-CGA
31	a1	405	CLA	C8-C10-C11-C12
38	B	625	DGA	CA2-CA3-CA4-CA5
41	g	624	LHG	C16-C17-C18-C19
41	N1	624	LHG	C17-C18-C19-C20
51	S	625	LPX	C12-C13-C14-C15
41	d	408	LHG	C10-C11-C12-C13
31	c	503	CLA	C16-C17-C18-C19
31	n	613	CLA	C16-C17-C18-C20
31	a1	410	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	s	608	CHL	C11-C12-C13-C14
41	c1	525	LHG	C16-C17-C18-C19
33	D	404	BCR	C11-C12-C13-C35
33	A1	411	BCR	C11-C12-C13-C35
33	B1	618	BCR	C7-C8-C9-C34
44	d	405	PL9	C2-C3-C7-C8
41	D1	410	LHG	C29-C30-C31-C32
41	G1	624	LHG	C14-C15-C16-C17
54	I1	102	4RF	C53-C54-C55-C56
31	C	512	CLA	C5-C6-C7-C8
31	n1	604	CLA	C10-C11-C12-C13
38	c	524	DGA	CA2-CA3-CA4-CA5
52	s	626	3PH	C34-C35-C36-C37
35	B	622	LMG	C29-C30-C31-C32
54	I1	102	4RF	C29-C30-C31-C32
35	b	622	LMG	C9-C8-O7-C10
40	b1	623	DGD	C1G-C2G-O2G-C1B
31	Y	603	CLA	C5-C6-C7-C8
31	y1	613	CLA	C4-C3-C5-C6
31	B	605	CLA	C1A-C2A-CAA-CBA
31	C	512	CLA	C1A-C2A-CAA-CBA
31	D	403	CLA	C1A-C2A-CAA-CBA
31	N	612	CLA	C1A-C2A-CAA-CBA
31	R	609	CLA	C1A-C2A-CAA-CBA
31	Y	611	CLA	C1A-C2A-CAA-CBA
31	c	506	CLA	C1A-C2A-CAA-CBA
31	n	613	CLA	C1A-C2A-CAA-CBA
31	B1	610	CLA	C1A-C2A-CAA-CBA
31	C1	502	CLA	C1A-C2A-CAA-CBA
31	Y1	602	CLA	C1A-C2A-CAA-CBA
31	c1	502	CLA	C1A-C2A-CAA-CBA
31	d1	403	CLA	C1A-C2A-CAA-CBA
31	y1	604	CLA	C1A-C2A-CAA-CBA
31	y1	610	CLA	C1A-C2A-CAA-CBA
47	N	608	CHL	C1A-C2A-CAA-CBA
47	n	608	CHL	C1A-C2A-CAA-CBA
47	n1	601	CHL	C1A-C2A-CAA-CBA
34	C	526	SQD	C31-C32-C33-C34
38	B	625	DGA	CB2-CB3-CB4-CB5
31	B	603	CLA	C12-C13-C15-C16
31	B	605	CLA	C11-C12-C13-C15
31	C	508	CLA	C12-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	609	CLA	C11-C10-C8-C7
31	R	610	CLA	C6-C7-C8-C10
31	Y	604	CLA	C11-C10-C8-C7
31	Y	613	CLA	C6-C7-C8-C10
31	b	607	CLA	C12-C13-C15-C16
31	d	402	CLA	C11-C10-C8-C7
31	y	611	CLA	C11-C10-C8-C7
31	C1	506	CLA	C11-C10-C8-C7
31	N1	603	CLA	C11-C10-C8-C7
31	G1	611	CLA	C6-C7-C8-C10
31	Y1	602	CLA	C12-C13-C15-C16
31	b1	610	CLA	C11-C12-C13-C15
31	c1	503	CLA	C6-C7-C8-C10
31	n1	613	CLA	C2-C3-C5-C6
47	Y1	606	CHL	C12-C13-C15-C16
47	y1	607	CHL	C11-C10-C8-C7
31	y	613	CLA	C13-C15-C16-C17
31	s1	614	CLA	O1A-CGA-O2A-C1
48	R1	620	LUT	C9-C10-C11-C12
41	C	525	LHG	C28-C29-C30-C31
41	d1	410	LHG	C34-C35-C36-C37
35	c1	523	LMG	C28-C29-C30-C31
31	b	610	CLA	O1A-CGA-O2A-C1
47	S	601	CHL	CAA-CBA-CGA-O2A
38	C	524	DGA	CA9-CAA-CBA-CCA
41	g1	624	LHG	C34-C35-C36-C37
31	A	405	CLA	C8-C10-C11-C12
31	c1	513	CLA	C15-C16-C17-C18
38	c	524	DGA	CBB-CAB-CB9-CB8
54	i1	101	4RF	C06-C07-C08-C09
31	B	610	CLA	C3-C5-C6-C7
31	S	602	CLA	C2A-CAA-CBA-CGA
31	a	406	CLA	C2A-CAA-CBA-CGA
31	r	608	CLA	C2A-CAA-CBA-CGA
31	r	613	CLA	C2A-CAA-CBA-CGA
31	s	613	CLA	C2A-CAA-CBA-CGA
31	B1	607	CLA	C2A-CAA-CBA-CGA
31	c1	510	CLA	C2A-CAA-CBA-CGA
31	s1	605	CLA	C2A-CAA-CBA-CGA
31	C	506	CLA	C15-C16-C17-C18
31	G	613	CLA	C15-C16-C17-C18
31	b1	609	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	s1	611	CLA	C5-C6-C7-C8
47	y	607	CHL	C10-C11-C12-C13
35	C	521	LMG	C39-C40-C41-C42
41	c	625	LHG	C30-C31-C32-C33
41	n	624	LHG	C16-C17-C18-C19
41	s1	624	LHG	C25-C26-C27-C28
47	s1	608	CHL	CAA-CBA-CGA-O2A
40	B1	623	DGD	C4A-C5A-C6A-C7A
41	d1	410	LHG	C31-C32-C33-C34
47	N	609	CHL	C8-C10-C11-C12
34	a1	412	SQD	C16-C17-C18-C19
31	b	602	CLA	C16-C17-C18-C20
31	S1	609	CLA	C5-C6-C7-C8
34	A	412	SQD	C11-C12-C13-C14
41	c1	525	LHG	C12-C13-C14-C15
53	Y	625	SPH	C11-C12-C13-C14
31	R	603	CLA	C4-C3-C5-C6
31	s	614	CLA	C4-C3-C5-C6
47	Y	609	CHL	C4-C3-C5-C6
38	B	625	DGA	CCA-CDA-CEA-CFA
41	g1	624	LHG	C29-C30-C31-C32
54	k1	101	4RF	C13-C14-C15-C16
31	n	602	CLA	C2-C3-C5-C6
40	c	523	DGD	O6D-C5D-C6D-O5D
47	S	601	CHL	CAA-CBA-CGA-O1A
47	R	606	CHL	C2A-CAA-CBA-CGA
31	G	610	CLA	C5-C6-C7-C8
31	y	611	CLA	C13-C15-C16-C17
31	G1	603	CLA	C10-C11-C12-C13
54	I1	102	4RF	C03-C04-C05-C06
34	C1	526	SQD	O49-C7-O47-C45
31	C	505	CLA	C16-C17-C18-C20
31	b	613	CLA	C16-C17-C18-C20
35	b1	622	LMG	C16-C17-C18-C19
33	D	404	BCR	C20-C21-C22-C23
33	d	404	BCR	C20-C21-C22-C23
50	r	623	NEX	C32-C33-C34-C35
50	y	623	NEX	C28-C29-C30-C31
50	G1	623	NEX	C28-C29-C30-C31
50	S1	623	NEX	C28-C29-C30-C31
31	a1	405	CLA	C5-C6-C7-C8
34	C	526	SQD	C13-C14-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	A	412	SQD	O47-C45-C46-O48
41	S	624	LHG	C33-C34-C35-C36
35	A	413	LMG	C29-C30-C31-C32
41	G	630	LHG	C33-C34-C35-C36
33	B	618	BCR	C13-C14-C15-C16
33	B	619	BCR	C13-C14-C15-C16
33	c	514	BCR	C19-C20-C21-C22
33	c	517	BCR	C19-C20-C21-C22
33	b1	618	BCR	C19-C20-C21-C22
33	c1	514	BCR	C19-C20-C21-C22
33	c1	517	BCR	C19-C20-C21-C22
48	Y	620	LUT	C33-C34-C35-C15
48	g1	621	LUT	C13-C14-C15-C35
49	R	621	XAT	C33-C34-C35-C15
31	R	610	CLA	C10-C11-C12-C13
31	C1	510	CLA	C8-C10-C11-C12
31	b1	603	CLA	C5-C6-C7-C8
41	G	630	LHG	C11-C12-C13-C14
31	B1	616	CLA	C16-C17-C18-C20
31	C1	509	CLA	C16-C17-C18-C20
54	K1	101	4RF	C48-C49-C50-C51
35	B	622	LMG	C19-C20-C21-C22
38	C1	524	DGA	CFA-CGA-CHA-CIA
31	s1	614	CLA	CBA-CGA-O2A-C1
41	d	410	LHG	C1-C2-C3-O3
51	s	625	LPX	C12-C13-C14-C15
47	Y	607	CHL	C13-C15-C16-C17
31	B	616	CLA	C4-C3-C5-C6
31	y	602	CLA	C4-C3-C5-C6
47	G1	601	CHL	C4-C3-C5-C6
47	g1	601	CHL	C4-C3-C5-C6
34	B1	626	SQD	C9-C10-C11-C12
35	a	413	LMG	C30-C31-C32-C33
35	B1	622	LMG	C11-C12-C13-C14
31	S	610	CLA	C2-C1-O2A-CGA
31	S	611	CLA	C2-C1-O2A-CGA
31	S	613	CLA	C2-C1-O2A-CGA
31	B1	610	CLA	C2-C1-O2A-CGA
31	b1	606	CLA	C2-C1-O2A-CGA
31	c1	513	CLA	C2-C1-O2A-CGA
47	N	609	CHL	C2-C1-O2A-CGA
47	n	608	CHL	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	N1	609	CHL	C2-C1-O2A-CGA
47	G1	606	CHL	C2-C1-O2A-CGA
47	Y1	609	CHL	C2-C1-O2A-CGA
31	s	604	CLA	C2-C3-C5-C6
31	C1	506	CLA	C2-C3-C5-C6
45	f	101	HEM	C2A-CAA-CBA-CGA
47	n	609	CHL	C2-C3-C5-C6
35	h1	102	LMG	C16-C17-C18-C19
32	A	408	PHO	C8-C10-C11-C12
34	A	412	SQD	O47-C7-C8-C9
35	D1	411	LMG	C10-C11-C12-C13
31	C	504	CLA	C6-C7-C8-C9
31	C	511	CLA	C11-C10-C8-C9
31	b	611	CLA	C11-C12-C13-C14
31	s	603	CLA	C6-C7-C8-C9
31	r1	610	CLA	C11-C10-C8-C9
47	N	609	CHL	C14-C13-C15-C16
41	D	409	LHG	C32-C33-C34-C35
35	h1	102	LMG	O10-C28-O8-C9
34	M1	101	SQD	C10-C11-C12-C13
41	D1	410	LHG	C33-C34-C35-C36
41	G1	624	LHG	C15-C16-C17-C18
31	Y1	614	CLA	C15-C16-C17-C18
35	a1	413	LMG	C11-C10-O7-C8
34	M1	101	SQD	O47-C7-C8-C9
35	B1	622	LMG	C13-C14-C15-C16
41	D1	408	LHG	O2-C2-C3-O3
31	b	616	CLA	C13-C15-C16-C17
31	c1	511	CLA	C5-C6-C7-C8
31	C	512	CLA	C2A-CAA-CBA-CGA
31	S1	614	CLA	C2A-CAA-CBA-CGA
31	n1	611	CLA	C2A-CAA-CBA-CGA
31	g1	611	CLA	C2A-CAA-CBA-CGA
47	N1	608	CHL	C2A-CAA-CBA-CGA
31	s1	612	CLA	CAA-CBA-CGA-O2A
41	d	410	LHG	C27-C28-C29-C30
31	n	602	CLA	O1A-CGA-O2A-C1
31	n1	613	CLA	O1A-CGA-O2A-C1
33	c	517	BCR	C1-C6-C7-C8
33	b1	619	BCR	C23-C24-C25-C30
33	c1	515	BCR	C1-C6-C7-C8
46	h	101	RRX	C23-C24-C25-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
46	H1	101	RRX	C23-C24-C25-C30
48	N	620	LUT	C1-C6-C7-C8
48	s	620	LUT	C1-C6-C7-C8
48	y	620	LUT	C1-C6-C7-C8
48	S1	620	LUT	C1-C6-C7-C8
48	Y1	620	LUT	C1-C6-C7-C8
48	Y1	620	LUT	C5-C6-C7-C8
48	g1	620	LUT	C1-C6-C7-C8
48	g1	620	LUT	C5-C6-C7-C8
47	S1	608	CHL	C10-C11-C12-C13
31	c	513	CLA	CAA-CBA-CGA-O2A
34	b1	621	SQD	O47-C7-C8-C9
35	a	413	LMG	C13-C14-C15-C16
35	a	413	LMG	C31-C32-C33-C34
35	C1	523	LMG	O1-C7-C8-C9
38	j1	101	DGA	CB3-CB4-CB5-CB6
40	C1	518	DGD	O1G-C1G-C2G-C3G
31	B1	615	CLA	C15-C16-C17-C18
39	b	624	GOL	C1-C2-C3-O3
34	a	412	SQD	C26-C27-C28-C29
31	b1	605	CLA	CAA-CBA-CGA-O1A
33	d	404	BCR	C9-C10-C11-C12
33	c1	516	BCR	C13-C14-C15-C16
37	B	620	C7Z	C33-C34-C35-C15
48	G1	620	LUT	C9-C10-C11-C12
48	y1	620	LUT	C29-C30-C31-C32
50	N	623	NEX	C33-C34-C35-C15
50	g1	623	NEX	C29-C30-C31-C32
38	B	625	DGA	CBA-CCA-CDA-CEA
31	c	504	CLA	C4-C3-C5-C6
31	r	608	CLA	C4-C3-C5-C6
44	d1	405	PL9	C15-C14-C16-C17
33	C1	514	BCR	C11-C12-C13-C14
31	B1	615	CLA	C16-C17-C18-C20
31	S	603	CLA	C13-C15-C16-C17
31	a	406	CLA	C5-C6-C7-C8
31	y1	604	CLA	C13-C15-C16-C17
31	c	506	CLA	C2-C3-C5-C6
31	C1	512	CLA	C2-C3-C5-C6
44	d1	405	PL9	C13-C14-C16-C17
31	D	402	CLA	C3-C5-C6-C7
31	R1	609	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	N	601	CHL	C3-C5-C6-C7
35	w1	201	LMG	O9-C10-C11-C12
31	S1	611	CLA	O1A-CGA-O2A-C1
42	C	527	LMK	C8-C9-O8-C28
49	n1	622	XAT	C14-C15-C35-C34
41	c1	525	LHG	C34-C35-C36-C37
35	B1	622	LMG	C33-C34-C35-C36
47	n	609	CHL	C4C-C3C-CAC-CBC
31	R	612	CLA	CAA-CBA-CGA-O2A
41	G1	624	LHG	O8-C23-C24-C25
54	k1	101	4RF	C07-C08-C09-C10
31	Y	611	CLA	C16-C17-C18-C20
31	b	612	CLA	C16-C17-C18-C19
31	C1	510	CLA	C16-C17-C18-C20
31	N1	610	CLA	C16-C17-C18-C20
38	B	625	DGA	CA7-CA8-CA9-CAA
41	L1	101	LHG	C30-C31-C32-C33
31	Y1	602	CLA	C5-C6-C7-C8
31	s1	602	CLA	C5-C6-C7-C8
41	Y1	624	LHG	O6-C4-C5-O7
52	b1	624	3PH	O11-C1-C2-O21
31	s	612	CLA	CAA-CBA-CGA-O2A
31	N1	612	CLA	CAA-CBA-CGA-O2A
31	S1	612	CLA	CAA-CBA-CGA-O2A
47	y	605	CHL	CAA-CBA-CGA-O2A
31	B	613	CLA	C2A-CAA-CBA-CGA
53	a1	414	SPH	C9-C10-C11-C12
31	S	614	CLA	CAA-CBA-CGA-O2A
41	N1	624	LHG	O8-C23-C24-C25
41	N1	624	LHG	C24-C23-O8-C6
54	k1	101	4RF	C33-C34-C35-C36
31	b1	612	CLA	C8-C10-C11-C12
52	S1	626	3PH	C3B-C3C-C3D-C3E
54	i1	101	4RF	C03-C04-C05-C06
31	b1	613	CLA	C3-C5-C6-C7
31	c	502	CLA	C16-C17-C18-C20
41	g	624	LHG	C10-C11-C12-C13
52	S1	626	3PH	C39-C3A-C3B-C3C
35	H1	102	LMG	O6-C1-O1-C7
38	C1	524	DGA	CEB-CFB-CGB-CHB
41	s	624	LHG	O6-C4-C5-C6
41	Y1	624	LHG	O6-C4-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	d1	410	LHG	O6-C4-C5-C6
52	b1	624	3PH	O11-C1-C2-C3
52	t1	101	3PH	O11-C1-C2-C3
38	c1	524	DGA	CA1-CA2-CA3-CA4
31	b	617	CLA	C4-C3-C5-C6
31	c	502	CLA	C4-C3-C5-C6
31	c	511	CLA	C4-C3-C5-C6
31	R1	609	CLA	C4-C3-C5-C6
47	N	605	CHL	C4-C3-C5-C6
41	d1	408	LHG	C8-C7-O7-C5
44	d	405	PL9	C24-C26-C27-C28
35	c1	521	LMG	O9-C10-C11-C12
40	C1	518	DGD	C9B-CAB-CBB-CCB
41	L	101	LHG	C26-C27-C28-C29
41	G	630	LHG	C34-C35-C36-C37
31	B	607	CLA	C11-C10-C8-C7
31	C	506	CLA	C6-C7-C8-C10
31	G	603	CLA	C6-C7-C8-C10
31	Y	603	CLA	C6-C7-C8-C10
31	b	611	CLA	C11-C10-C8-C7
31	b	614	CLA	C2-C3-C5-C6
31	c	506	CLA	C11-C12-C13-C15
31	c	507	CLA	C11-C12-C13-C15
31	s	602	CLA	C11-C10-C8-C7
31	s	610	CLA	C6-C7-C8-C10
31	y	613	CLA	C11-C10-C8-C7
31	B1	605	CLA	C12-C13-C15-C16
31	C1	510	CLA	C11-C12-C13-C15
31	S1	603	CLA	C11-C12-C13-C15
31	b1	607	CLA	C12-C13-C15-C16
31	b1	608	CLA	C11-C12-C13-C15
31	b1	615	CLA	C6-C7-C8-C10
31	c1	507	CLA	C6-C7-C8-C10
31	n1	604	CLA	C2-C3-C5-C6
31	g1	610	CLA	C11-C12-C13-C15
31	s1	603	CLA	C2-C3-C5-C6
31	y1	604	CLA	C12-C13-C15-C16
44	d1	405	PL9	C28-C29-C31-C32
47	y	606	CHL	C2-C3-C5-C6
47	g1	601	CHL	C2-C3-C5-C6
35	h1	102	LMG	C29-C28-O8-C9
31	r	609	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	C1	524	DGA	CFB-CGB-CHB-CIB
57	Y1	626	PTY	C19-C20-C21-C22
41	Y	624	LHG	O1-C1-C2-O2
41	Y1	624	LHG	O1-C1-C2-O2
41	c1	525	LHG	O1-C1-C2-O2
41	d	408	LHG	C14-C15-C16-C17
38	J1	101	DGA	OG2-CG2-CG3-OXT
38	c1	524	DGA	OG2-CG2-CG3-OXT
47	g	601	CHL	C5-C6-C7-C8
48	n1	620	LUT	C29-C30-C31-C32
31	c1	505	CLA	CAA-CBA-CGA-O2A
34	M1	101	SQD	C2-C1-O6-C44
41	s1	624	LHG	C10-C11-C12-C13
41	S1	624	LHG	C5-C4-O6-P
34	B	621	SQD	O47-C45-C46-O48
34	C	526	SQD	O6-C44-C45-O47
34	a	412	SQD	O6-C44-C45-O47
35	c	521	LMG	O7-C8-C9-O8
40	c	519	DGD	O1G-C1G-C2G-O2G
41	y1	624	LHG	O7-C5-C6-O8
31	G1	612	CLA	C2A-CAA-CBA-CGA
31	B1	613	CLA	C8-C10-C11-C12
47	y	605	CHL	CAA-CBA-CGA-O1A
47	n	608	CHL	O2A-C1-C2-C3
47	r	607	CHL	O2A-C1-C2-C3
47	R1	607	CHL	O2A-C1-C2-C3
31	y1	613	CLA	CAA-CBA-CGA-O2A
38	B1	625	DGA	OG2-CB1-CB2-CB3
41	n1	624	LHG	O7-C7-C8-C9
35	c1	523	LMG	C30-C31-C32-C33
41	D	408	LHG	C10-C11-C12-C13
47	G	606	CHL	C2A-CAA-CBA-CGA
47	Y	609	CHL	C2A-CAA-CBA-CGA
31	c	509	CLA	C5-C6-C7-C8
31	b1	602	CLA	C15-C16-C17-C18
31	B	609	CLA	C16-C17-C18-C19
31	C	502	CLA	C16-C17-C18-C20
31	Y	603	CLA	C16-C17-C18-C19
31	B1	605	CLA	C16-C17-C18-C19
44	D1	405	PL9	C2-C3-C7-C8
41	L	101	LHG	C8-C7-O7-C5
31	B1	609	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	G	602	CLA	C10-C11-C12-C13
34	A	412	SQD	C11-C10-C9-C8
35	c1	523	LMG	C11-C12-C13-C14
50	N	623	NEX	C40-C33-C34-C35
50	n	623	NEX	C39-C29-C30-C31
50	y	623	NEX	C39-C29-C30-C31
31	y	613	CLA	CAA-CBA-CGA-O2A
31	S1	610	CLA	CAA-CBA-CGA-O2A
57	y1	626	PTY	O4-C30-C31-C32
31	s	609	CLA	C4-C3-C5-C6
31	S1	610	CLA	C4-C3-C5-C6
31	b1	602	CLA	C4-C3-C5-C6
31	y1	614	CLA	C4-C3-C5-C6
32	a1	409	PHO	C4-C3-C5-C6
44	d	405	PL9	C45-C44-C46-C47
47	y	609	CHL	C4-C3-C5-C6
47	n1	609	CHL	C4-C3-C5-C6
47	g1	607	CHL	C4-C3-C5-C6
31	a	406	CLA	C15-C16-C17-C18
31	C1	509	CLA	C13-C15-C16-C17
31	c1	512	CLA	C13-C15-C16-C17
41	d	409	LHG	C25-C26-C27-C28
31	B	610	CLA	C2-C3-C5-C6
31	R	603	CLA	C2-C3-C5-C6
31	b	605	CLA	C2-C3-C5-C6
31	y1	613	CLA	C2-C3-C5-C6
41	C	525	LHG	C9-C10-C11-C12
41	d	410	LHG	C34-C35-C36-C37
41	d1	409	LHG	C31-C32-C33-C34
31	n	602	CLA	CBA-CGA-O2A-C1
38	b	623	DGA	OG2-CB1-CB2-CB3
38	c	524	DGA	OG1-CA1-CA2-CA3
38	b1	625	DGA	OG2-CB1-CB2-CB3
40	C	518	DGD	O6D-C5D-C6D-O5D
35	d1	411	LMG	C22-C23-C24-C25
31	B	607	CLA	C11-C10-C8-C9
31	B	607	CLA	C14-C13-C15-C16
31	B	613	CLA	C11-C12-C13-C14
31	N	610	CLA	C11-C12-C13-C14
31	R	609	CLA	C11-C10-C8-C9
31	b	605	CLA	C11-C12-C13-C14
31	b	616	CLA	C6-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	501	CLA	C6-C7-C8-C9
31	y	602	CLA	C14-C13-C15-C16
31	A1	406	CLA	C11-C12-C13-C14
31	B1	602	CLA	C14-C13-C15-C16
31	B1	605	CLA	C14-C13-C15-C16
31	B1	607	CLA	C11-C12-C13-C14
31	C1	512	CLA	C11-C10-C8-C9
31	N1	603	CLA	C11-C10-C8-C9
31	N1	613	CLA	C14-C13-C15-C16
31	G1	602	CLA	C14-C13-C15-C16
31	S1	611	CLA	C6-C7-C8-C9
31	Y1	613	CLA	C6-C7-C8-C9
31	g1	610	CLA	C14-C13-C15-C16
47	Y	609	CHL	C11-C12-C13-C14
47	n	606	CHL	C11-C12-C13-C14
47	y	607	CHL	C6-C7-C8-C9
47	G1	607	CHL	C11-C12-C13-C14
47	n1	605	CHL	C14-C13-C15-C16
47	s1	608	CHL	C11-C10-C8-C9
47	y1	607	CHL	C11-C10-C8-C9
34	B	621	SQD	C11-C10-C9-C8
40	c1	519	DGD	C2A-C3A-C4A-C5A
53	A1	414	SPH	C11-C10-C9-C8
31	N1	612	CLA	CAA-CBA-CGA-O1A
47	s	601	CHL	CAA-CBA-CGA-O2A
47	s1	601	CHL	CAA-CBA-CGA-O2A
31	B	613	CLA	C3A-C2A-CAA-CBA
31	R	610	CLA	C3A-C2A-CAA-CBA
31	c	501	CLA	C3A-C2A-CAA-CBA
31	c	513	CLA	C3A-C2A-CAA-CBA
31	n	610	CLA	C3A-C2A-CAA-CBA
31	n	614	CLA	C3A-C2A-CAA-CBA
31	s	605	CLA	C3A-C2A-CAA-CBA
31	s	612	CLA	C3A-C2A-CAA-CBA
47	N	608	CHL	C3A-C2A-CAA-CBA
47	G1	601	CHL	C3A-C2A-CAA-CBA
47	G1	607	CHL	C3A-C2A-CAA-CBA
47	n1	607	CHL	C3A-C2A-CAA-CBA
52	s	626	3PH	C28-C29-C2A-C2B
31	Y	613	CLA	CAA-CBA-CGA-O2A
31	b	603	CLA	CAA-CBA-CGA-O2A
31	b	608	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	d1	402	CLA	CAA-CBA-CGA-O2A
34	c1	526	SQD	O47-C7-C8-C9
40	C1	520	DGD	O2G-C1B-C2B-C3B
53	Y	625	SPH	C4-C5-C6-C7
53	a1	414	SPH	C4-C5-C6-C7
35	B	622	LMG	C14-C15-C16-C17
35	J	101	LMG	C32-C33-C34-C35
35	j	101	LMG	C12-C13-C14-C15
31	B	613	CLA	CAD-CBD-CGD-O2D
31	C	509	CLA	CAD-CBD-CGD-O2D
31	N	602	CLA	CAD-CBD-CGD-O2D
31	G	604	CLA	CAD-CBD-CGD-O2D
31	G	614	CLA	CAD-CBD-CGD-O2D
31	S	611	CLA	CAD-CBD-CGD-O2D
31	Y	602	CLA	CAD-CBD-CGD-O2D
31	b	617	CLA	CAD-CBD-CGD-O2D
31	n	602	CLA	CAD-CBD-CGD-O2D
31	n	610	CLA	CAD-CBD-CGD-O2D
31	s	614	CLA	CAD-CBD-CGD-O2D
31	A1	407	CLA	CAD-CBD-CGD-O2D
31	C1	509	CLA	CAD-CBD-CGD-O2D
31	C1	512	CLA	CAD-CBD-CGD-O2D
31	N1	602	CLA	CAD-CBD-CGD-O2D
31	N1	603	CLA	CAD-CBD-CGD-O2D
31	G1	602	CLA	CAD-CBD-CGD-O2D
31	G1	603	CLA	CAD-CBD-CGD-O2D
31	G1	614	CLA	CAD-CBD-CGD-O2D
31	S1	604	CLA	CAD-CBD-CGD-O2D
31	S1	611	CLA	CAD-CBD-CGD-O2D
31	b1	606	CLA	CAD-CBD-CGD-O2D
31	b1	607	CLA	CAD-CBD-CGD-O2D
31	b1	617	CLA	CAD-CBD-CGD-O2D
31	c1	512	CLA	CAD-CBD-CGD-O2D
31	g1	614	CLA	CAD-CBD-CGD-O2D
31	r1	612	CLA	CAD-CBD-CGD-O2D
32	A	408	PHO	CAD-CBD-CGD-O2D
32	A1	409	PHO	CAD-CBD-CGD-O2D
35	b	622	LMG	C7-C8-O7-C10
42	c	627	LMK	C1-C2-C3-N4
47	R	606	CHL	CAD-CBD-CGD-O2D
47	Y	605	CHL	CAD-CBD-CGD-O2D
47	Y	607	CHL	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	n	601	CHL	CAD-CBD-CGD-O2D
47	s	608	CHL	CAD-CBD-CGD-O2D
47	Y1	606	CHL	CAD-CBD-CGD-O2D
47	n1	605	CHL	CAD-CBD-CGD-O2D
47	g1	607	CHL	CAD-CBD-CGD-O2D
47	s1	608	CHL	CAD-CBD-CGD-O2D
31	y	602	CLA	C16-C17-C18-C20
47	R1	606	CHL	C2A-CAA-CBA-CGA
54	K1	101	4RF	C46-C47-C48-C49
54	k1	101	4RF	C09-C10-C11-C12
31	C1	503	CLA	C15-C16-C17-C18
50	r1	622	NEX	C33-C34-C35-C15
40	c1	520	DGD	C4A-C5A-C6A-C7A
41	d1	409	LHG	C9-C10-C11-C12
31	y	604	CLA	C5-C6-C7-C8
31	d1	403	CLA	C2-C1-O2A-CGA
31	n1	612	CLA	CAA-CBA-CGA-O2A
34	b1	626	SQD	C35-C36-C37-C38
52	s	626	3PH	C32-C33-C34-C35
52	B1	624	3PH	C22-C23-C24-C25
41	s1	624	LHG	C7-C8-C9-C10
31	A	405	CLA	CAA-CBA-CGA-O2A
31	G	614	CLA	CAA-CBA-CGA-O2A
35	J	101	LMG	O7-C10-C11-C12
35	W1	201	LMG	O7-C10-C11-C12
38	C1	524	DGA	OG2-CB1-CB2-CB3
38	b1	625	DGA	OG1-CA1-CA2-CA3
41	D1	409	LHG	O7-C7-C8-C9
47	n1	605	CHL	CAA-CBA-CGA-O2A
51	s1	625	LPX	O6-C6-C7-C8
52	B1	624	3PH	O31-C31-C32-C33
34	m1	101	SQD	C28-C29-C30-C31
41	d1	410	LHG	C24-C25-C26-C27
31	B	607	CLA	C15-C16-C17-C18
42	c1	527	LMK	C10-C11-C12-C13
31	A1	406	CLA	C4-C3-C5-C6
31	C1	513	CLA	C4-C3-C5-C6
31	c1	505	CLA	C4-C3-C5-C6
44	D1	405	PL9	C45-C44-C46-C47
44	d1	405	PL9	C45-C44-C46-C47
31	g1	613	CLA	C16-C17-C18-C19
31	C	508	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	S1	612	CLA	CAA-CBA-CGA-O1A
31	s1	612	CLA	CAA-CBA-CGA-O1A
35	B	622	LMG	C18-C19-C20-C21
31	s	614	CLA	C2-C3-C5-C6
31	A1	406	CLA	C2-C3-C5-C6
47	Y	609	CHL	C2-C3-C5-C6
47	N1	609	CHL	C2-C3-C5-C6
31	B	602	CLA	CAA-CBA-CGA-O2A
31	B1	603	CLA	CAA-CBA-CGA-O2A
31	B1	615	CLA	CAA-CBA-CGA-O2A
31	R1	604	CLA	CAA-CBA-CGA-O2A
31	r1	612	CLA	CAA-CBA-CGA-O2A
32	A1	409	PHO	CAA-CBA-CGA-O2A
35	j	101	LMG	O7-C10-C11-C12
35	H1	102	LMG	O7-C10-C11-C12
41	d	410	LHG	O8-C23-C24-C25
40	c	519	DGD	C7B-C8B-C9B-CAB
33	C	516	BCR	C11-C12-C13-C14
33	A1	411	BCR	C11-C12-C13-C14
33	B1	618	BCR	C7-C8-C9-C10
48	g	620	LUT	C27-C28-C29-C30
49	R	621	XAT	C31-C32-C33-C34
31	Y	602	CLA	C15-C16-C17-C18
42	c	627	LMK	C11-C10-O7-C8
49	r	622	XAT	O24-C26-C27-C28
49	y1	622	XAT	O24-C26-C27-C28
50	y1	623	NEX	O24-C26-C27-C28
52	i	101	3PH	C1-C2-C3-O31
52	t1	101	3PH	C1-C2-C3-O31
52	s1	626	3PH	C1-O11-P-O12
31	s	612	CLA	CAA-CBA-CGA-O1A
47	s	601	CHL	CAA-CBA-CGA-O1A
31	C1	501	CLA	O1A-CGA-O2A-C1
47	n	607	CHL	C10-C11-C12-C13
31	S1	602	CLA	C3-C5-C6-C7
31	B	608	CLA	CAA-CBA-CGA-O2A
31	r	610	CLA	CAA-CBA-CGA-O2A
31	Y1	613	CLA	CAA-CBA-CGA-O2A
54	I1	102	4RF	O40-C41-C43-C44
31	g1	611	CLA	C16-C17-C18-C20
41	Y	624	LHG	C33-C34-C35-C36
41	n	624	LHG	C19-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	L1	101	LHG	C29-C30-C31-C32
52	b1	624	3PH	C3D-C3E-C3F-C3G
53	Y1	625	SPH	C10-C11-C12-C13
47	R	607	CHL	O2A-C1-C2-C3
47	g	606	CHL	O2A-C1-C2-C3
31	A1	405	CLA	CAA-CBA-CGA-O1A
41	n	624	LHG	O10-C23-C24-C25
47	s1	601	CHL	CAA-CBA-CGA-O1A
34	A1	412	SQD	C10-C11-C12-C13
38	c1	524	DGA	CA3-CA4-CA5-CA6
31	B	617	CLA	C15-C16-C17-C18
31	A	405	CLA	O2A-C1-C2-C3
47	G1	609	CHL	O2A-C1-C2-C3
47	g1	601	CHL	O2A-C1-C2-C3
35	D	411	LMG	C14-C15-C16-C17
35	H	102	LMG	C16-C17-C18-C19
41	n1	624	LHG	C30-C31-C32-C33
51	S	625	LPX	C7-C8-C9-C10
31	b	603	CLA	C2A-CAA-CBA-CGA
41	d1	408	LHG	C35-C36-C37-C38
41	D	410	LHG	O8-C23-C24-C25
41	Y	624	LHG	O8-C23-C24-C25
41	S1	624	LHG	O8-C23-C24-C25
52	s1	626	3PH	O21-C21-C22-C23
31	b1	603	CLA	C3-C5-C6-C7
31	B1	609	CLA	O1A-CGA-O2A-C1
38	b	623	DGA	CCB-CDB-CEB-CFB
52	s	626	3PH	C38-C39-C3A-C3B
40	c	519	DGD	CCB-CDB-CEB-CFB
31	B	608	CLA	CHA-CBD-CGD-O1D
31	B	608	CLA	CHA-CBD-CGD-O2D
31	B	611	CLA	CHA-CBD-CGD-O1D
31	B	611	CLA	CHA-CBD-CGD-O2D
31	C	504	CLA	CHA-CBD-CGD-O1D
31	C	507	CLA	CHA-CBD-CGD-O1D
31	C	507	CLA	CHA-CBD-CGD-O2D
31	D	402	CLA	CHA-CBD-CGD-O2D
31	N	610	CLA	CHA-CBD-CGD-O1D
31	N	610	CLA	CHA-CBD-CGD-O2D
31	N	612	CLA	CHA-CBD-CGD-O2D
31	G	603	CLA	CHA-CBD-CGD-O2D
31	R	608	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	609	CLA	CHA-CBD-CGD-O2D
31	S	604	CLA	CHA-CBD-CGD-O1D
31	S	604	CLA	CHA-CBD-CGD-O2D
31	S	609	CLA	CHA-CBD-CGD-O1D
31	S	609	CLA	CHA-CBD-CGD-O2D
31	S	611	CLA	CHA-CBD-CGD-O1D
31	S	611	CLA	CHA-CBD-CGD-O2D
31	S	612	CLA	CHA-CBD-CGD-O1D
31	S	612	CLA	CHA-CBD-CGD-O2D
31	Y	603	CLA	CHA-CBD-CGD-O2D
31	Y	610	CLA	CHA-CBD-CGD-O1D
31	Y	610	CLA	CHA-CBD-CGD-O2D
31	b	602	CLA	CHA-CBD-CGD-O1D
31	b	602	CLA	CHA-CBD-CGD-O2D
31	b	606	CLA	CHA-CBD-CGD-O2D
31	b	614	CLA	CHA-CBD-CGD-O1D
31	b	614	CLA	CHA-CBD-CGD-O2D
31	c	502	CLA	CHA-CBD-CGD-O2D
31	c	505	CLA	CHA-CBD-CGD-O2D
31	c	506	CLA	CHA-CBD-CGD-O1D
31	c	506	CLA	CHA-CBD-CGD-O2D
31	c	507	CLA	CHA-CBD-CGD-O1D
31	c	507	CLA	CHA-CBD-CGD-O2D
31	c	509	CLA	CHA-CBD-CGD-O1D
31	c	511	CLA	CHA-CBD-CGD-O1D
31	c	511	CLA	CHA-CBD-CGD-O2D
31	g	602	CLA	CHA-CBD-CGD-O1D
31	g	602	CLA	CHA-CBD-CGD-O2D
31	g	603	CLA	CHA-CBD-CGD-O2D
31	r	604	CLA	CHA-CBD-CGD-O2D
31	r	608	CLA	CHA-CBD-CGD-O1D
31	r	608	CLA	CHA-CBD-CGD-O2D
31	s	603	CLA	CHA-CBD-CGD-O1D
31	s	603	CLA	CHA-CBD-CGD-O2D
31	s	609	CLA	CHA-CBD-CGD-O1D
31	s	609	CLA	CHA-CBD-CGD-O2D
31	s	617	CLA	CHA-CBD-CGD-O2D
31	y	603	CLA	CHA-CBD-CGD-O1D
31	y	603	CLA	CHA-CBD-CGD-O2D
31	y	604	CLA	CHA-CBD-CGD-O1D
31	y	604	CLA	CHA-CBD-CGD-O2D
31	y	608	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	A1	405	CLA	CHA-CBD-CGD-O1D
31	A1	405	CLA	CHA-CBD-CGD-O2D
31	B1	602	CLA	CHA-CBD-CGD-O1D
31	B1	602	CLA	CHA-CBD-CGD-O2D
31	B1	611	CLA	CHA-CBD-CGD-O2D
31	B1	616	CLA	CHA-CBD-CGD-O1D
31	B1	616	CLA	CHA-CBD-CGD-O2D
31	C1	507	CLA	CHA-CBD-CGD-O1D
31	C1	507	CLA	CHA-CBD-CGD-O2D
31	N1	604	CLA	CHA-CBD-CGD-O2D
31	N1	613	CLA	CHA-CBD-CGD-O1D
31	N1	613	CLA	CHA-CBD-CGD-O2D
31	G1	610	CLA	CHA-CBD-CGD-O1D
31	G1	610	CLA	CHA-CBD-CGD-O2D
31	R1	612	CLA	CHA-CBD-CGD-O1D
31	R1	612	CLA	CHA-CBD-CGD-O2D
31	S1	611	CLA	CHA-CBD-CGD-O2D
31	S1	613	CLA	CHA-CBD-CGD-O1D
31	S1	613	CLA	CHA-CBD-CGD-O2D
31	Y1	602	CLA	CHA-CBD-CGD-O1D
31	Y1	602	CLA	CHA-CBD-CGD-O2D
31	Y1	603	CLA	CHA-CBD-CGD-O1D
31	Y1	603	CLA	CHA-CBD-CGD-O2D
31	Y1	604	CLA	CHA-CBD-CGD-O1D
31	Y1	604	CLA	CHA-CBD-CGD-O2D
31	Y1	610	CLA	CHA-CBD-CGD-O1D
31	Y1	610	CLA	CHA-CBD-CGD-O2D
31	a1	405	CLA	CHA-CBD-CGD-O1D
31	a1	405	CLA	CHA-CBD-CGD-O2D
31	a1	407	CLA	CHA-CBD-CGD-O2D
31	b1	608	CLA	CHA-CBD-CGD-O1D
31	b1	608	CLA	CHA-CBD-CGD-O2D
31	b1	610	CLA	CHA-CBD-CGD-O2D
31	b1	611	CLA	CHA-CBD-CGD-O1D
31	b1	611	CLA	CHA-CBD-CGD-O2D
31	b1	614	CLA	CHA-CBD-CGD-O1D
31	b1	614	CLA	CHA-CBD-CGD-O2D
31	c1	505	CLA	CHA-CBD-CGD-O1D
31	c1	510	CLA	CHA-CBD-CGD-O1D
31	c1	510	CLA	CHA-CBD-CGD-O2D
31	n1	603	CLA	CHA-CBD-CGD-O1D
31	n1	610	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	n1	610	CLA	CHA-CBD-CGD-O2D
31	n1	612	CLA	CHA-CBD-CGD-O2D
31	n1	613	CLA	CHA-CBD-CGD-O2D
31	g1	603	CLA	CHA-CBD-CGD-O2D
31	g1	604	CLA	CHA-CBD-CGD-O1D
31	r1	608	CLA	CHA-CBD-CGD-O1D
31	r1	608	CLA	CHA-CBD-CGD-O2D
31	r1	609	CLA	CHA-CBD-CGD-O1D
31	r1	609	CLA	CHA-CBD-CGD-O2D
31	s1	610	CLA	CHA-CBD-CGD-O1D
31	s1	610	CLA	CHA-CBD-CGD-O2D
31	s1	612	CLA	CHA-CBD-CGD-O1D
31	s1	612	CLA	CHA-CBD-CGD-O2D
31	y1	602	CLA	CHA-CBD-CGD-O1D
31	y1	604	CLA	CHA-CBD-CGD-O1D
31	y1	604	CLA	CHA-CBD-CGD-O2D
31	y1	613	CLA	CHA-CBD-CGD-O1D
31	y1	613	CLA	CHA-CBD-CGD-O2D
47	N	601	CHL	CHA-CBD-CGD-O1D
47	N	608	CHL	CHA-CBD-CGD-O1D
47	N	608	CHL	CHA-CBD-CGD-O2D
47	G	605	CHL	CHA-CBD-CGD-O1D
47	G	605	CHL	CHA-CBD-CGD-O2D
47	G	606	CHL	CHA-CBD-CGD-O1D
47	G	606	CHL	CHA-CBD-CGD-O2D
47	G	609	CHL	CHA-CBD-CGD-O1D
47	G	609	CHL	CHA-CBD-CGD-O2D
47	y	609	CHL	CHA-CBD-CGD-O2D
47	G1	601	CHL	CHA-CBD-CGD-O1D
47	G1	601	CHL	CHA-CBD-CGD-O2D
47	R1	606	CHL	CHA-CBD-CGD-O1D
47	S1	607	CHL	CHA-CBD-CGD-O1D
47	S1	607	CHL	CHA-CBD-CGD-O2D
47	S1	608	CHL	CHA-CBD-CGD-O1D
47	S1	608	CHL	CHA-CBD-CGD-O2D
47	n1	609	CHL	CHA-CBD-CGD-O1D
47	n1	609	CHL	CHA-CBD-CGD-O2D
47	g1	608	CHL	CHA-CBD-CGD-O1D
47	g1	608	CHL	CHA-CBD-CGD-O2D
47	s1	607	CHL	CHA-CBD-CGD-O2D
47	y1	609	CHL	CHA-CBD-CGD-O1D
47	y1	609	CHL	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
48	G	621	LUT	C9-C10-C11-C12
48	N1	621	LUT	C9-C10-C11-C12
31	c	501	CLA	C13-C15-C16-C17
31	C1	503	CLA	CAA-CBA-CGA-O2A
31	g1	603	CLA	CAA-CBA-CGA-O2A
35	W1	201	LMG	O8-C28-C29-C30
41	D	408	LHG	O7-C7-C8-C9
34	A1	412	SQD	C26-C27-C28-C29
38	c	524	DGA	CEA-CFA-CGA-CHA
41	l	101	LHG	C29-C30-C31-C32
41	n1	624	LHG	C31-C32-C33-C34
41	d	410	LHG	C29-C30-C31-C32
41	Y	624	LHG	O6-C4-C5-C6
52	s1	626	3PH	O11-C1-C2-C3
50	N	623	NEX	C12-C13-C14-C15
50	N	623	NEX	C28-C29-C30-C31
50	n	623	NEX	C28-C29-C30-C31
31	b1	609	CLA	C10-C11-C12-C13
31	B	609	CLA	CAA-CBA-CGA-O2A
31	N	604	CLA	CAA-CBA-CGA-O2A
31	c	503	CLA	CAA-CBA-CGA-O2A
31	s	611	CLA	CAA-CBA-CGA-O2A
31	s	614	CLA	CAA-CBA-CGA-O2A
31	b1	608	CLA	CAA-CBA-CGA-O2A
31	b1	610	CLA	CAA-CBA-CGA-O2A
31	b1	613	CLA	CAA-CBA-CGA-O2A
31	c1	503	CLA	CAA-CBA-CGA-O2A
35	c	521	LMG	O7-C10-C11-C12
41	y	624	LHG	O8-C23-C24-C25
41	g1	624	LHG	O8-C23-C24-C25
41	L1	101	LHG	C9-C10-C11-C12
41	n1	624	LHG	C11-C10-C9-C8
35	H1	102	LMG	O7-C8-C9-O8
40	C	519	DGD	O2G-C2G-C3G-O3G
52	t1	101	3PH	O21-C2-C3-O31
40	B1	623	DGD	C3A-C4A-C5A-C6A
52	s1	626	3PH	C22-C23-C24-C25
31	R	610	CLA	C5-C6-C7-C8
31	Y1	612	CLA	C15-C16-C17-C18
31	g1	603	CLA	C5-C6-C7-C8
34	b	621	SQD	C29-C30-C31-C32
41	d1	409	LHG	C26-C27-C28-C29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
55	R1	625	LMT	C9-C10-C11-C12
47	y	607	CHL	C13-C15-C16-C17
31	R	610	CLA	CAA-CBA-CGA-O2A
31	B1	608	CLA	CAA-CBA-CGA-O2A
31	C1	512	CLA	CAA-CBA-CGA-O2A
34	a1	412	SQD	O47-C7-C8-C9
35	d	411	LMG	O7-C10-C11-C12
38	C	524	DGA	OG1-CA1-CA2-CA3
40	C1	518	DGD	O1G-C1A-C2A-C3A
41	y1	624	LHG	O8-C23-C24-C25
31	r1	608	CLA	C2A-CAA-CBA-CGA
32	A	409	PHO	C2A-CAA-CBA-CGA
32	a	408	PHO	CHA-CBD-CGD-O1D
32	a	409	PHO	CHA-CBD-CGD-O1D
42	C1	527	LMK	O9-C10-C11-C12
31	b1	616	CLA	C10-C11-C12-C13
31	g1	613	CLA	C10-C11-C12-C13
31	S1	611	CLA	CBA-CGA-O2A-C1
34	C1	526	SQD	C24-C23-O48-C46
47	S	606	CHL	C2A-CAA-CBA-CGA
34	C1	526	SQD	C8-C7-O47-C45
31	C1	505	CLA	CAA-CBA-CGA-O2A
31	G1	603	CLA	CAA-CBA-CGA-O2A
31	c1	508	CLA	CAA-CBA-CGA-O2A
41	N1	624	LHG	O7-C7-C8-C9
52	S1	626	3PH	O21-C21-C22-C23
41	d1	409	LHG	C29-C30-C31-C32
35	A1	413	LMG	C4-C5-C6-O5
31	B	610	CLA	C6-C7-C8-C10
31	B	613	CLA	C11-C12-C13-C15
31	B	616	CLA	C6-C7-C8-C10
31	N	602	CLA	C12-C13-C15-C16
31	R	608	CLA	C11-C10-C8-C7
31	c	507	CLA	C6-C7-C8-C10
31	R1	602	CLA	C6-C7-C8-C10
31	S1	602	CLA	C6-C7-C8-C10
31	Y1	603	CLA	C11-C10-C8-C7
31	b1	605	CLA	C12-C13-C15-C16
31	b1	614	CLA	C6-C7-C8-C10
31	g1	610	CLA	C6-C7-C8-C10
31	y1	603	CLA	C11-C10-C8-C7
44	D1	405	PL9	C12-C11-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	N	607	CHL	C11-C12-C13-C15
47	Y	609	CHL	C11-C12-C13-C15
47	n	605	CHL	C11-C10-C8-C7
47	n1	609	CHL	C2-C3-C5-C6
31	b1	608	CLA	C16-C17-C18-C19
31	b1	611	CLA	C16-C17-C18-C20
41	L	101	LHG	C2-C3-O3-P
41	N1	624	LHG	C2-C3-O3-P
52	T1	101	3PH	C2-C1-O11-P
35	C1	523	LMG	C31-C32-C33-C34
52	s	626	3PH	C2E-C2F-C2G-C2H
31	B	612	CLA	CAA-CBA-CGA-O2A
31	C	503	CLA	CAA-CBA-CGA-O2A
35	c1	523	LMG	O7-C10-C11-C12
41	N	624	LHG	O8-C23-C24-C25
35	C1	521	LMG	C12-C13-C14-C15
40	C1	519	DGD	C2B-C3B-C4B-C5B
31	B	610	CLA	C6-C7-C8-C9
31	B	614	CLA	C11-C12-C13-C14
31	C	508	CLA	C14-C13-C15-C16
31	R	608	CLA	C11-C10-C8-C9
31	R	610	CLA	C6-C7-C8-C9
31	Y	604	CLA	C6-C7-C8-C9
31	Y	610	CLA	C6-C7-C8-C9
31	b	607	CLA	C11-C12-C13-C14
31	d	402	CLA	C11-C10-C8-C9
31	s	610	CLA	C6-C7-C8-C9
31	y	611	CLA	C11-C10-C8-C9
31	R1	603	CLA	C11-C10-C8-C9
31	S1	602	CLA	C6-C7-C8-C9
31	Y1	602	CLA	C14-C13-C15-C16
31	b1	605	CLA	C14-C13-C15-C16
31	b1	606	CLA	C11-C12-C13-C14
31	c1	507	CLA	C6-C7-C8-C9
31	d1	402	CLA	C11-C12-C13-C14
31	n1	602	CLA	C11-C12-C13-C14
31	s1	610	CLA	C6-C7-C8-C9
31	s1	611	CLA	C11-C12-C13-C14
47	n1	606	CHL	C11-C10-C8-C9
33	b1	618	BCR	C13-C14-C15-C16
48	N	621	LUT	C33-C34-C35-C15
49	r1	621	XAT	C29-C30-C31-C32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	a1	412	SQD	C14-C15-C16-C17
40	c1	520	DGD	C3A-C4A-C5A-C6A
31	n1	611	CLA	O2A-C1-C2-C3
47	g1	606	CHL	O2A-C1-C2-C3
38	b	623	DGA	CB4-CB5-CB6-CB7
35	b1	622	LMG	C14-C15-C16-C17
31	n1	613	CLA	CBA-CGA-O2A-C1
31	n1	613	CLA	C8-C10-C11-C12
31	n	613	CLA	CAA-CBA-CGA-O2A
31	b1	615	CLA	CAA-CBA-CGA-O2A
31	y1	613	CLA	CAA-CBA-CGA-O1A
35	C1	521	LMG	O9-C10-C11-C12
34	A	412	SQD	C4-C5-C6-S
34	b	621	SQD	C4-C5-C6-S
34	C1	526	SQD	C4-C5-C6-S
34	b1	621	SQD	C4-C5-C6-S
34	c1	526	SQD	C4-C5-C6-S
35	A1	413	LMG	C33-C34-C35-C36
34	C1	526	SQD	O10-C23-O48-C46
35	h	102	LMG	O10-C28-O8-C9
38	B	625	DGA	CDB-CEB-CFB-CGB
41	L	101	LHG	C17-C18-C19-C20
41	s	624	LHG	C24-C25-C26-C27
41	d1	409	LHG	C15-C16-C17-C18
47	g1	605	CHL	C2-C1-O2A-CGA
31	Y	610	CLA	C10-C11-C12-C13
41	l	101	LHG	C8-C7-O7-C5
31	G1	602	CLA	C2A-CAA-CBA-CGA
35	J	101	LMG	O9-C10-C11-C12
31	n	604	CLA	CAA-CBA-CGA-O2A
31	g1	613	CLA	CAA-CBA-CGA-O2A
41	d1	408	LHG	O7-C7-C8-C9
35	C	521	LMG	C30-C31-C32-C33
38	b1	625	DGA	CA7-CA8-CA9-CAA
35	C1	523	LMG	C11-C12-C13-C14
31	n1	612	CLA	CAA-CBA-CGA-O1A
31	y	613	CLA	CAA-CBA-CGA-O1A
31	S1	610	CLA	CAA-CBA-CGA-O1A
54	I1	102	4RF	O42-C41-C43-C44
31	b1	609	CLA	C5-C6-C7-C8
31	c1	512	CLA	C15-C16-C17-C18
52	s	626	3PH	C3C-C3D-C3E-C3F

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	y	604	CLA	C4-C3-C5-C6
38	C	524	DGA	CEA-CFA-CGA-CHA
41	N1	624	LHG	O10-C23-O8-C6
31	c	502	CLA	C2-C3-C5-C6
31	g	610	CLA	C2-C3-C5-C6
31	B	603	CLA	CAA-CBA-CGA-O2A
31	b	602	CLA	CAA-CBA-CGA-O2A
40	C	519	DGD	C5A-C6A-C7A-C8A
40	c	518	DGD	CCB-CDB-CEB-CFB
41	n1	624	LHG	C19-C20-C21-C22
31	A	405	CLA	CAA-CBA-CGA-O1A
31	B	602	CLA	CAA-CBA-CGA-O1A
31	r	610	CLA	CAA-CBA-CGA-O1A
32	A1	409	PHO	CAA-CBA-CGA-O1A
38	c	524	DGA	OA1-CA1-CA2-CA3
38	B1	625	DGA	OB1-CB1-CB2-CB3
37	B	620	C7Z	C11-C12-C13-C14
48	g	621	LUT	C27-C28-C29-C30
34	a1	412	SQD	C15-C16-C17-C18
35	c	521	LMG	C32-C33-C34-C35
31	B	616	CLA	C13-C15-C16-C17
31	B	613	CLA	C1A-C2A-CAA-CBA
31	B	617	CLA	C1A-C2A-CAA-CBA
31	C	506	CLA	C1A-C2A-CAA-CBA
31	N	604	CLA	C1A-C2A-CAA-CBA
31	Y	608	CLA	C1A-C2A-CAA-CBA
31	b	613	CLA	C1A-C2A-CAA-CBA
31	b	616	CLA	C1A-C2A-CAA-CBA
31	c	513	CLA	C1A-C2A-CAA-CBA
31	s	612	CLA	C1A-C2A-CAA-CBA
31	s	614	CLA	C1A-C2A-CAA-CBA
31	B1	615	CLA	C1A-C2A-CAA-CBA
31	R1	603	CLA	C1A-C2A-CAA-CBA
31	S1	614	CLA	C1A-C2A-CAA-CBA
31	b1	611	CLA	C1A-C2A-CAA-CBA
31	s1	614	CLA	C1A-C2A-CAA-CBA
31	y1	602	CLA	C1A-C2A-CAA-CBA
31	y1	613	CLA	C1A-C2A-CAA-CBA
47	G	601	CHL	C1A-C2A-CAA-CBA
47	y	601	CHL	C1A-C2A-CAA-CBA
47	N1	606	CHL	C1A-C2A-CAA-CBA
47	N1	609	CHL	C1A-C2A-CAA-CBA

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	Y1	606	CHL	C1A-C2A-CAA-CBA
47	n1	605	CHL	C1A-C2A-CAA-CBA
47	y1	609	CHL	C1A-C2A-CAA-CBA
34	B	621	SQD	C17-C18-C19-C20
41	D	408	LHG	C27-C28-C29-C30
31	c1	512	CLA	C16-C17-C18-C20
31	R1	604	CLA	CAA-CBA-CGA-O1A
34	c1	526	SQD	O49-C7-C8-C9
35	j	101	LMG	O9-C10-C11-C12
38	b1	625	DGA	OB1-CB1-CB2-CB3
40	C1	520	DGD	O1B-C1B-C2B-C3B
41	d	410	LHG	O10-C23-C24-C25
31	n	611	CLA	CAA-CBA-CGA-O2A
53	y	625	SPH	C4-C5-C6-C7
31	Y	602	CLA	C2-C1-O2A-CGA
31	Y	613	CLA	C2-C1-O2A-CGA
34	C1	526	SQD	C12-C13-C14-C15
54	k1	101	4RF	C08-C09-C10-C11
31	B1	615	CLA	CAA-CBA-CGA-O1A
31	c1	505	CLA	CAA-CBA-CGA-O1A
31	r1	612	CLA	CAA-CBA-CGA-O1A
41	D1	409	LHG	O9-C7-C8-C9
57	y1	626	PTY	O30-C30-C31-C32
34	a	412	SQD	C32-C33-C34-C35
52	S1	626	3PH	C28-C29-C2A-C2B
41	n	624	LHG	C4-C5-C6-O8
54	I1	102	4RF	O18-C19-C20-C39
40	c1	518	DGD	O1G-C1A-C2A-C3A
52	s	626	3PH	O21-C21-C22-C23
41	n1	624	LHG	C18-C19-C20-C21
52	S1	626	3PH	C3F-C3G-C3H-C3I
31	s1	603	CLA	C2A-CAA-CBA-CGA
31	s1	610	CLA	C2A-CAA-CBA-CGA
41	s	624	LHG	C35-C36-C37-C38
41	y	624	LHG	C9-C10-C11-C12
53	Y	625	SPH	C12-C13-C14-C15
57	y1	626	PTY	C21-C22-C23-C24
40	c	520	DGD	O6D-C5D-C6D-O5D
41	D	410	LHG	O2-C2-C3-O3
31	C1	512	CLA	CAA-CBA-CGA-O1A
38	b	623	DGA	OB1-CB1-CB2-CB3
41	n1	624	LHG	O9-C7-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	n1	605	CHL	CAA-CBA-CGA-O1A
51	s1	625	LPX	O7-C6-C7-C8
31	Y	613	CLA	C10-C11-C12-C13
35	b	622	LMG	C21-C22-C23-C24
34	B1	626	SQD	C28-C29-C30-C31
41	G	630	LHG	C35-C36-C37-C38
47	S1	606	CHL	C2A-CAA-CBA-CGA
56	r1	626	ERG	C22-C23-C24-C25
31	S	617	CLA	CAA-CBA-CGA-O2A
31	b	612	CLA	CAA-CBA-CGA-O2A
31	g	614	CLA	CAA-CBA-CGA-O2A
31	G1	614	CLA	CAA-CBA-CGA-O2A
31	b1	609	CLA	CAA-CBA-CGA-O2A
47	g1	605	CHL	CAA-CBA-CGA-O2A
31	Y	613	CLA	C13-C15-C16-C17
47	S1	608	CHL	C3-C5-C6-C7
40	C	518	DGD	C4D-C5D-C6D-O5D
35	b	622	LMG	C15-C16-C17-C18
40	C	519	DGD	CDB-CEB-CFB-CGB
31	R	610	CLA	CAA-CBA-CGA-O1A
31	Y1	613	CLA	CAA-CBA-CGA-O1A
35	W1	201	LMG	O9-C10-C11-C12
38	C1	524	DGA	OB1-CB1-CB2-CB3
41	D	408	LHG	O9-C7-C8-C9
40	c1	520	DGD	O6D-C5D-C6D-O5D
34	m1	101	SQD	C10-C11-C12-C13
41	n1	624	LHG	C24-C25-C26-C27
31	b1	603	CLA	C8-C10-C11-C12
41	D	409	LHG	C35-C36-C37-C38
41	d	408	LHG	C35-C36-C37-C38
47	n	609	CHL	C2C-C3C-CAC-CBC
41	D	409	LHG	C4-O6-P-O5
41	N	624	LHG	C3-O3-P-O5
41	G	630	LHG	C3-O3-P-O5
41	S	624	LHG	C3-O3-P-O4
41	Y	624	LHG	C3-O3-P-O5
41	d	409	LHG	C3-O3-P-O5
41	d	409	LHG	C4-O6-P-O5
41	n	624	LHG	C3-O3-P-O5
41	g	624	LHG	C3-O3-P-O5
41	L1	101	LHG	C4-O6-P-O5
41	N1	624	LHG	C3-O3-P-O5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
41	Y1	624	LHG	C3-O3-P-O5
34	m1	101	SQD	C23-C24-C25-C26
31	B1	603	CLA	CAA-CBA-CGA-O1A
31	C1	503	CLA	CAA-CBA-CGA-O1A
31	b1	610	CLA	CAA-CBA-CGA-O1A
31	g1	603	CLA	CAA-CBA-CGA-O1A
35	c1	523	LMG	O9-C10-C11-C12
38	b1	625	DGA	OA1-CA1-CA2-CA3
41	Y	624	LHG	O10-C23-C24-C25
41	y	624	LHG	O10-C23-C24-C25
41	S1	624	LHG	O10-C23-C24-C25
31	N	611	CLA	O2A-C1-C2-C3
41	g	624	LHG	C27-C28-C29-C30
53	y	625	SPH	C13-C14-C15-C16
33	A	411	BCR	C1-C6-C7-C8
33	A	411	BCR	C5-C6-C7-C8
33	C	514	BCR	C23-C24-C25-C30
33	b1	619	BCR	C23-C24-C25-C26
48	N	620	LUT	C5-C6-C7-C8
48	y	620	LUT	C5-C6-C7-C8
48	y1	620	LUT	C1-C6-C7-C8
35	a1	413	LMG	C33-C34-C35-C36
31	B	611	CLA	C8-C10-C11-C12
49	R	621	XAT	C26-C27-C28-C29
49	G1	622	XAT	C26-C27-C28-C29
31	B	608	CLA	CAA-CBA-CGA-O1A
31	G	614	CLA	CAA-CBA-CGA-O1A
31	Y	613	CLA	CAA-CBA-CGA-O1A
31	b	603	CLA	CAA-CBA-CGA-O1A
31	c	503	CLA	CAA-CBA-CGA-O1A
31	s	614	CLA	CAA-CBA-CGA-O1A
31	b1	608	CLA	CAA-CBA-CGA-O1A
31	b1	615	CLA	CAA-CBA-CGA-O1A
35	c	521	LMG	O9-C10-C11-C12
41	D	410	LHG	O10-C23-C24-C25
41	y1	624	LHG	O10-C23-C24-C25
52	B1	624	3PH	O32-C31-C32-C33
31	B	610	CLA	CAA-CBA-CGA-O2A
31	B1	609	CLA	CAA-CBA-CGA-O2A
31	c1	512	CLA	CAA-CBA-CGA-O2A
35	C1	523	LMG	O7-C10-C11-C12
47	R	607	CHL	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	G1	607	CHL	CAA-CBA-CGA-O2A
47	y1	606	CHL	CAA-CBA-CGA-O2A
31	B1	615	CLA	C8-C10-C11-C12
31	c1	511	CLA	C13-C15-C16-C17
31	B	612	CLA	C16-C17-C18-C20
40	c1	518	DGD	C4A-C5A-C6A-C7A
47	G	609	CHL	C2C-C3C-CAC-CBC
49	Y	622	XAT	C30-C31-C32-C33
31	G1	603	CLA	C2A-CAA-CBA-CGA
31	b	608	CLA	CAA-CBA-CGA-O1A
31	c1	503	CLA	CAA-CBA-CGA-O1A
35	d	411	LMG	O9-C10-C11-C12
35	W1	201	LMG	O10-C28-C29-C30
31	s	609	CLA	C3-C5-C6-C7
34	B1	626	SQD	C27-C28-C29-C30
38	b1	625	DGA	CA2-CA3-CA4-CA5
41	G	630	LHG	C32-C33-C34-C35
41	n	624	LHG	C33-C34-C35-C36
31	s	603	CLA	CAA-CBA-CGA-O2A
47	r1	607	CHL	CAA-CBA-CGA-O2A
54	K1	101	4RF	O40-C41-C43-C44
31	Y	604	CLA	C13-C15-C16-C17
31	C1	510	CLA	C13-C15-C16-C17
41	D1	408	LHG	C35-C36-C37-C38
41	N1	624	LHG	C16-C17-C18-C19
31	N	604	CLA	CAA-CBA-CGA-O1A
34	a1	412	SQD	O49-C7-C8-C9
31	b1	607	CLA	C4-C3-C5-C6
44	D1	405	PL9	C12-C11-C9-C10
31	s1	610	CLA	C2-C3-C5-C6
34	C	526	SQD	C11-C12-C13-C14
57	Y1	626	PTY	C15-C16-C17-C18
31	B	606	CLA	CAD-CBD-CGD-O1D
31	B	616	CLA	CAD-CBD-CGD-O1D
31	C	510	CLA	CAD-CBD-CGD-O1D
31	C	513	CLA	CAD-CBD-CGD-O1D
31	N	604	CLA	CAD-CBD-CGD-O1D
31	b	612	CLA	CAD-CBD-CGD-O1D
31	b	614	CLA	CAD-CBD-CGD-O1D
31	c	513	CLA	CAD-CBD-CGD-O1D
31	s	611	CLA	CAD-CBD-CGD-O1D
31	s	617	CLA	CAD-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	y	608	CLA	CAD-CBD-CGD-O1D
31	B1	606	CLA	CAD-CBD-CGD-O1D
31	B1	613	CLA	CAD-CBD-CGD-O1D
31	S1	603	CLA	CAD-CBD-CGD-O1D
31	S1	617	CLA	CAD-CBD-CGD-O1D
31	c1	505	CLA	CAD-CBD-CGD-O1D
31	n1	614	CLA	CAD-CBD-CGD-O1D
34	b	621	SQD	O5-C5-C6-S
34	B1	621	SQD	O5-C5-C6-S
34	C1	526	SQD	O5-C5-C6-S
34	c1	526	SQD	O5-C5-C6-S
40	B1	623	DGD	C1G-C2G-O2G-C1B
40	b1	623	DGD	C3G-C2G-O2G-C1B
47	N	601	CHL	CAD-CBD-CGD-O1D
47	G	605	CHL	CAD-CBD-CGD-O1D
47	N1	601	CHL	CAD-CBD-CGD-O1D
47	S1	607	CHL	CAD-CBD-CGD-O1D
47	n1	609	CHL	CAD-CBD-CGD-O1D
57	y1	626	PTY	C2-C3-O11-P1
47	g	608	CHL	CBD-CGD-O2D-CED
34	C1	526	SQD	C23-C24-C25-C26
54	i1	101	4RF	C22-C24-C25-C26
31	B	603	CLA	CAA-CBA-CGA-O1A
31	B1	608	CLA	CAA-CBA-CGA-O1A
31	G1	603	CLA	CAA-CBA-CGA-O1A
34	m1	101	SQD	O49-C7-C8-C9
34	b	621	SQD	C11-C10-C9-C8
31	B	607	CLA	CAA-CBA-CGA-O2A
31	g	613	CLA	CAA-CBA-CGA-O2A
31	y	614	CLA	CAA-CBA-CGA-O2A
31	A1	406	CLA	CAA-CBA-CGA-O2A
31	s1	614	CLA	CAA-CBA-CGA-O2A
35	C	521	LMG	O7-C10-C11-C12
38	B	625	DGA	OG2-CB1-CB2-CB3
40	c1	518	DGD	O2G-C1B-C2B-C3B
41	d1	409	LHG	O7-C7-C8-C9
41	s1	624	LHG	O8-C23-C24-C25
31	s	609	CLA	C8-C10-C11-C12
31	A	406	CLA	C11-C12-C13-C14
31	B	605	CLA	C11-C12-C13-C14
31	C	501	CLA	C14-C13-C15-C16
31	b	607	CLA	C14-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	c	505	CLA	C14-C13-C15-C16
31	n	603	CLA	C11-C10-C8-C9
31	s	610	CLA	C11-C12-C13-C14
31	y	604	CLA	C6-C7-C8-C9
31	y	613	CLA	C6-C7-C8-C9
31	B1	603	CLA	C14-C13-C15-C16
31	C1	506	CLA	C11-C10-C8-C9
31	S1	603	CLA	C11-C12-C13-C14
31	Y1	604	CLA	C6-C7-C8-C9
31	b1	608	CLA	C11-C10-C8-C9
31	b1	613	CLA	C11-C12-C13-C14
31	b1	615	CLA	C11-C12-C13-C14
31	c1	501	CLA	C6-C7-C8-C9
31	c1	507	CLA	C11-C12-C13-C14
31	c1	508	CLA	C11-C12-C13-C14
31	g1	610	CLA	C11-C12-C13-C14
32	a1	408	PHO	C6-C7-C8-C9
47	N	606	CHL	C11-C12-C13-C14
47	n	607	CHL	C11-C12-C13-C14
47	g1	609	CHL	C11-C12-C13-C14
42	C	527	LMK	C30-C31-C32-C33
31	B	610	CLA	C5-C6-C7-C8
31	S	610	CLA	C10-C11-C12-C13
31	r1	609	CLA	C10-C11-C12-C13
35	H	102	LMG	O9-C10-C11-C12
35	A	413	LMG	C34-C35-C36-C37
35	D1	411	LMG	C11-C12-C13-C14
47	G	609	CHL	C3-C5-C6-C7
31	C	505	CLA	CAA-CBA-CGA-O2A
31	b	610	CLA	CAA-CBA-CGA-O2A
31	b	617	CLA	CAA-CBA-CGA-O2A
31	g	604	CLA	CAA-CBA-CGA-O2A
31	C1	508	CLA	CAA-CBA-CGA-O2A
31	C1	513	CLA	CAA-CBA-CGA-O2A
31	c1	513	CLA	CAA-CBA-CGA-O2A
41	D1	408	LHG	O8-C23-C24-C25
52	b1	624	3PH	O21-C21-C22-C23
38	C1	524	DGA	CA8-CA9-CAA-CBA
31	C	513	CLA	C13-C15-C16-C17
31	N1	610	CLA	C8-C10-C11-C12
41	S1	624	LHG	C33-C34-C35-C36
31	B	612	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	R	609	CLA	CAA-CBA-CGA-O1A
41	L	101	LHG	O9-C7-C8-C9
31	g	613	CLA	C5-C6-C7-C8
31	C	509	CLA	C2A-CAA-CBA-CGA
35	H1	102	LMG	C40-C41-C42-C43
31	C	508	CLA	CAA-CBA-CGA-O2A
31	G	613	CLA	CAA-CBA-CGA-O2A
31	g	603	CLA	CAA-CBA-CGA-O2A
31	B1	607	CLA	CAA-CBA-CGA-O2A
31	c1	502	CLA	CAA-CBA-CGA-O2A
31	n1	611	CLA	CAA-CBA-CGA-O2A
31	n1	614	CLA	CAA-CBA-CGA-O2A
31	r1	604	CLA	CAA-CBA-CGA-O2A
32	a1	409	PHO	CAA-CBA-CGA-O2A
34	B1	621	SQD	O47-C7-C8-C9
35	d1	411	LMG	O7-C10-C11-C12
38	C	524	DGA	OG2-CB1-CB2-CB3
40	C	523	DGD	O1G-C1A-C2A-C3A
41	D	408	LHG	O8-C23-C24-C25
41	c	625	LHG	O8-C23-C24-C25
41	c1	525	LHG	O7-C7-C8-C9
47	y	606	CHL	CAA-CBA-CGA-O2A
35	A	413	LMG	C11-C12-C13-C14
38	B1	625	DGA	CCB-CDB-CEB-CFB
31	B	609	CLA	CAA-CBA-CGA-O1A
31	C	503	CLA	CAA-CBA-CGA-O1A
31	C1	505	CLA	CAA-CBA-CGA-O1A
31	b1	613	CLA	CAA-CBA-CGA-O1A
31	c1	508	CLA	CAA-CBA-CGA-O1A
38	C	524	DGA	OA1-CA1-CA2-CA3
40	C1	518	DGD	O1A-C1A-C2A-C3A
31	y	613	CLA	C16-C17-C18-C19
31	Y	603	CLA	C4-C3-C5-C6
31	n	610	CLA	C4-C3-C5-C6
31	s	610	CLA	C4-C3-C5-C6
31	c1	513	CLA	C4-C3-C5-C6
31	b	609	CLA	C10-C11-C12-C13
31	B	616	CLA	C12-C13-C15-C16
31	C	504	CLA	C6-C7-C8-C10
31	C	511	CLA	C11-C10-C8-C7
31	G	602	CLA	C11-C10-C8-C7
31	S	611	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	Y	603	CLA	C11-C12-C13-C15
31	b	604	CLA	C12-C13-C15-C16
31	b	610	CLA	C2-C3-C5-C6
31	b	613	CLA	C6-C7-C8-C10
31	b	613	CLA	C11-C12-C13-C15
31	c	505	CLA	C12-C13-C15-C16
31	s	611	CLA	C12-C13-C15-C16
31	y	602	CLA	C11-C10-C8-C7
31	A1	406	CLA	C11-C12-C13-C15
31	B1	603	CLA	C11-C12-C13-C15
31	S1	602	CLA	C11-C10-C8-C7
31	Y1	602	CLA	C11-C10-C8-C7
31	Y1	603	CLA	C6-C7-C8-C10
31	a1	406	CLA	C11-C10-C8-C7
31	b1	602	CLA	C11-C12-C13-C15
31	b1	605	CLA	C11-C10-C8-C7
31	b1	606	CLA	C11-C12-C13-C15
31	b1	613	CLA	C11-C12-C13-C15
31	b1	615	CLA	C11-C12-C13-C15
31	b1	617	CLA	C12-C13-C15-C16
31	c1	506	CLA	C11-C10-C8-C7
31	c1	507	CLA	C11-C12-C13-C15
31	c1	512	CLA	C11-C12-C13-C15
31	r1	612	CLA	C6-C7-C8-C10
31	s1	611	CLA	C12-C13-C15-C16
32	a	408	PHO	C11-C12-C13-C15
32	a	409	PHO	C11-C10-C8-C7
32	a1	408	PHO	C6-C7-C8-C10
47	N1	606	CHL	C12-C13-C15-C16
47	y1	607	CHL	C6-C7-C8-C10
52	S1	626	3PH	C31-C32-C33-C34
31	b	612	CLA	CAA-CBA-CGA-O1A
31	n	611	CLA	CAA-CBA-CGA-O1A
31	s	610	CLA	CAA-CBA-CGA-O1A
31	c1	502	CLA	CAA-CBA-CGA-O1A
38	B	625	DGA	OB1-CB1-CB2-CB3
38	B1	625	DGA	OA1-CA1-CA2-CA3
41	N1	624	LHG	O9-C7-C8-C9
41	n1	624	LHG	O10-C23-C24-C25
47	g1	605	CHL	CAA-CBA-CGA-O1A
31	g	611	CLA	CAA-CBA-CGA-O2A
57	y1	626	PTY	C24-C25-C26-C27

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
40	C	520	DGD	O6D-C5D-C6D-O5D
31	B	605	CLA	CAA-CBA-CGA-O2A
31	b	609	CLA	CAA-CBA-CGA-O2A
31	c	501	CLA	CAA-CBA-CGA-O2A
31	n	603	CLA	CAA-CBA-CGA-O2A
31	s	610	CLA	CAA-CBA-CGA-O2A
31	g1	614	CLA	CAA-CBA-CGA-O2A
38	B	625	DGA	OG1-CA1-CA2-CA3
41	d	408	LHG	O8-C23-C24-C25
54	K1	101	4RF	C14-C15-C16-O18
31	y1	603	CLA	C8-C10-C11-C12
47	g1	608	CHL	C2A-CAA-CBA-CGA
34	A	412	SQD	C10-C11-C12-C13
41	N	624	LHG	C29-C30-C31-C32
31	d1	402	CLA	C3-C5-C6-C7
34	A	412	SQD	C27-C28-C29-C30
41	N	624	LHG	C23-C24-C25-C26
33	B	618	BCR	C7-C8-C9-C10
33	D	404	BCR	C11-C12-C13-C14
33	c	516	BCR	C11-C12-C13-C14
33	A1	411	BCR	C7-C8-C9-C10
33	C1	514	BCR	C21-C22-C23-C24
33	b1	619	BCR	C11-C12-C13-C14
33	c1	514	BCR	C11-C12-C13-C14
48	n	621	LUT	C31-C32-C33-C34
48	S1	621	LUT	C31-C32-C33-C34
49	n	622	XAT	C27-C28-C29-C30
50	Y	623	NEX	C11-C12-C13-C14
31	C	508	CLA	CAA-CBA-CGA-O1A
31	b	609	CLA	CAA-CBA-CGA-O1A
31	c	501	CLA	CAA-CBA-CGA-O1A
31	g1	613	CLA	CAA-CBA-CGA-O1A
35	C1	523	LMG	O9-C10-C11-C12
41	c1	525	LHG	O9-C7-C8-C9
41	d1	408	LHG	O9-C7-C8-C9
33	c1	514	BCR	C15-C16-C17-C18
48	n	621	LUT	C9-C10-C11-C12
52	b1	624	3PH	C3E-C3F-C3G-C3H
52	t1	101	3PH	C28-C29-C2A-C2B
31	b	602	CLA	C16-C17-C18-C19
31	c1	502	CLA	C16-C17-C18-C19
31	b1	602	CLA	CAA-CBA-CGA-O2A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
38	B1	625	DGA	OG1-CA1-CA2-CA3
52	t1	101	3PH	O31-C31-C32-C33
38	c	524	DGA	CAB-CBB-CCB-CDB
31	B	608	CLA	C15-C16-C17-C18
31	B1	602	CLA	C8-C10-C11-C12
31	Y1	604	CLA	C10-C11-C12-C13
32	a	409	PHO	C10-C11-C12-C13
38	c	524	DGA	OA1-CA1-OG1-CG1
52	T1	101	3PH	C21-C22-C23-C24
31	b	602	CLA	CAA-CBA-CGA-O1A
31	b	610	CLA	CAA-CBA-CGA-O1A
31	b	617	CLA	CAA-CBA-CGA-O1A
31	n	603	CLA	CAA-CBA-CGA-O1A
31	n	604	CLA	CAA-CBA-CGA-O1A
31	g	614	CLA	CAA-CBA-CGA-O1A
31	C1	513	CLA	CAA-CBA-CGA-O1A
31	G1	614	CLA	CAA-CBA-CGA-O1A
31	b1	609	CLA	CAA-CBA-CGA-O1A
34	B1	621	SQD	O49-C7-C8-C9
38	B	625	DGA	OA1-CA1-CA2-CA3
40	C	523	DGD	O1A-C1A-C2A-C3A
40	c1	518	DGD	O1A-C1A-C2A-C3A
47	y	606	CHL	CAA-CBA-CGA-O1A
52	s	626	3PH	O22-C21-C22-C23
52	b1	624	3PH	O22-C21-C22-C23
52	s1	626	3PH	O22-C21-C22-C23
54	K1	101	4RF	C14-C15-C16-O17
31	G	610	CLA	C8-C10-C11-C12
31	B1	607	CLA	C13-C15-C16-C17
31	N1	610	CLA	C5-C6-C7-C8
31	b1	611	CLA	C5-C6-C7-C8
41	d	410	LHG	O2-C2-C3-O3
31	D	402	CLA	CAA-CBA-CGA-O2A
31	G	603	CLA	CAA-CBA-CGA-O2A
31	R1	612	CLA	CAA-CBA-CGA-O2A
31	a1	406	CLA	CAA-CBA-CGA-O2A
38	J1	101	DGA	OG2-CB1-CB2-CB3
41	G	630	LHG	O8-C23-C24-C25
41	S1	624	LHG	O7-C7-C8-C9
47	g1	606	CHL	CAA-CBA-CGA-O2A
31	R	608	CLA	C10-C11-C12-C13
31	c1	505	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
47	n	607	CHL	C15-C16-C17-C18
31	G	613	CLA	CAA-CBA-CGA-O1A
31	S	617	CLA	CAA-CBA-CGA-O1A
31	g	613	CLA	CAA-CBA-CGA-O1A
31	n1	611	CLA	CAA-CBA-CGA-O1A
35	d1	411	LMG	O9-C10-C11-C12
31	c1	511	CLA	C16-C17-C18-C20
31	d	402	CLA	C5-C6-C7-C8
31	s	613	CLA	C5-C6-C7-C8
31	b1	617	CLA	C13-C15-C16-C17
32	a	408	PHO	C10-C11-C12-C13
47	N	605	CHL	C15-C16-C17-C18
31	g1	614	CLA	CAA-CBA-CGA-O1A
41	D	408	LHG	O10-C23-C24-C25
41	d	408	LHG	O10-C23-C24-C25
31	B	604	CLA	C4-C3-C5-C6
35	b1	622	LMG	C19-C20-C21-C22
41	y	624	LHG	C31-C32-C33-C34
54	i1	101	4RF	C35-C36-C37-C38
31	C	513	CLA	CAA-CBA-CGA-O2A
31	D1	402	CLA	CAA-CBA-CGA-O2A
34	b	621	SQD	O48-C23-C24-C25
35	h	102	LMG	O7-C10-C11-C12
38	c1	524	DGA	OG1-CA1-CA2-CA3

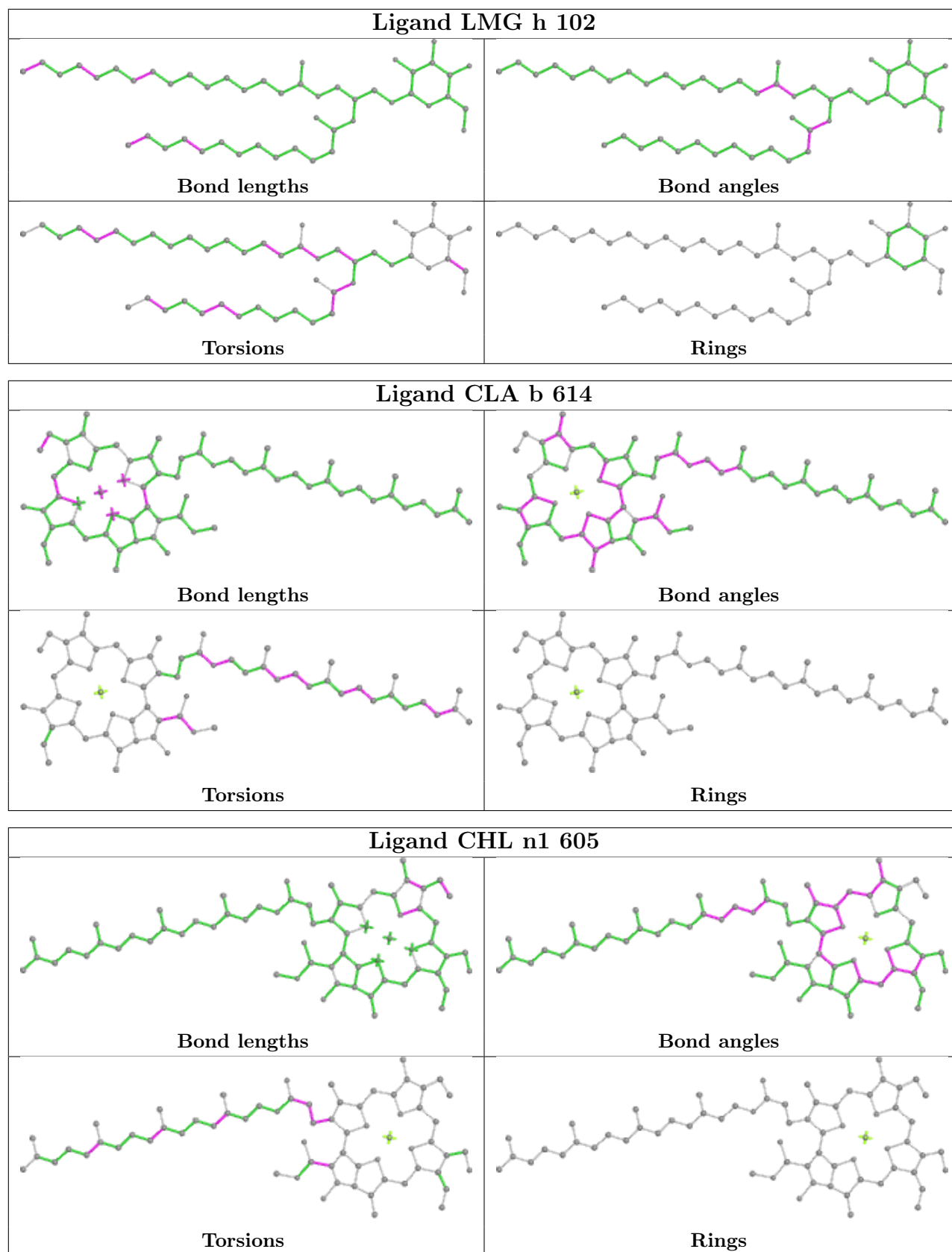
All (1) ring outliers are listed below:

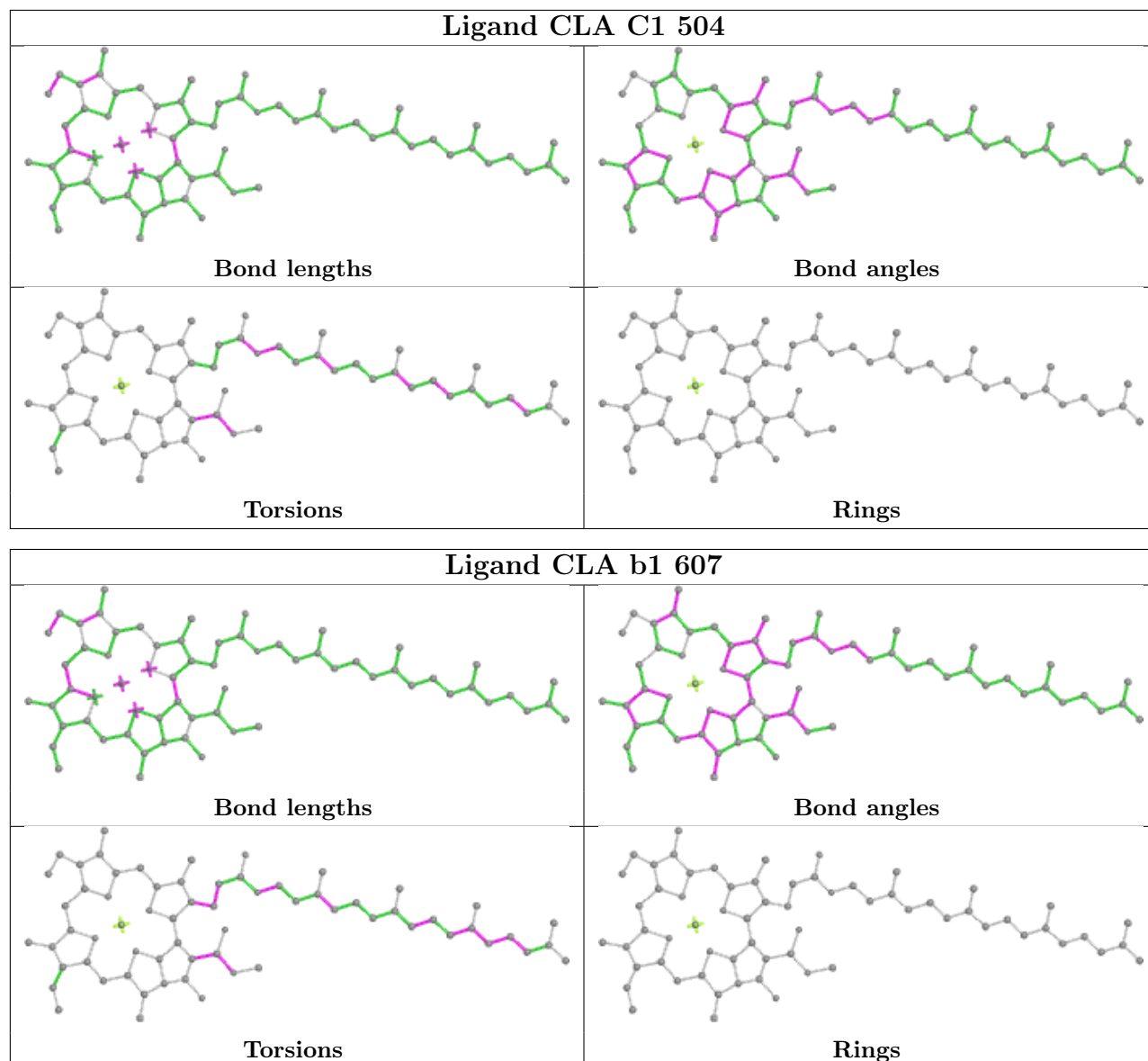
Mol	Chain	Res	Type	Atoms
50	n1	623	NEX	C1-C2-C3-C4-C5-C6

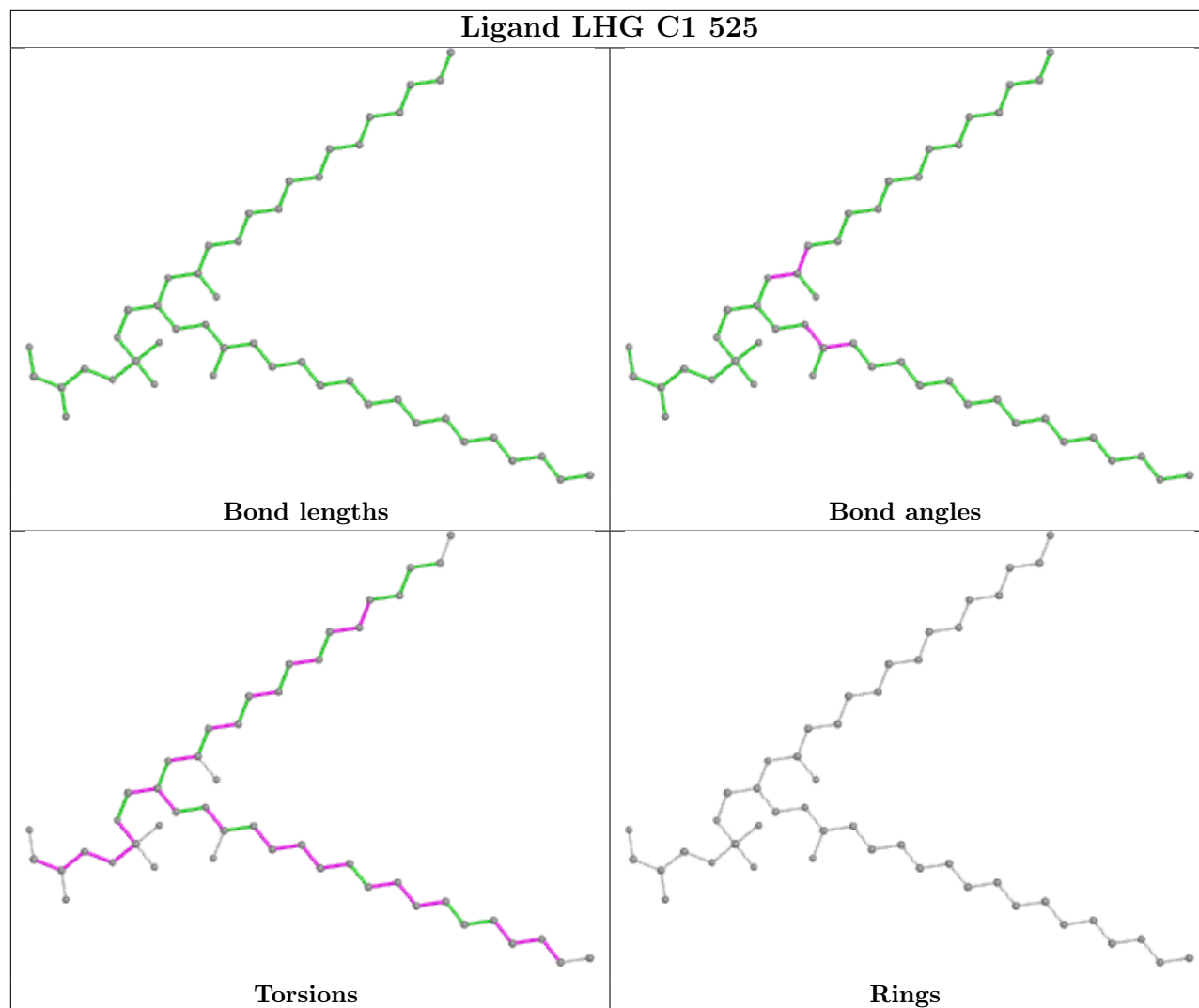
No monomer is involved in short contacts.

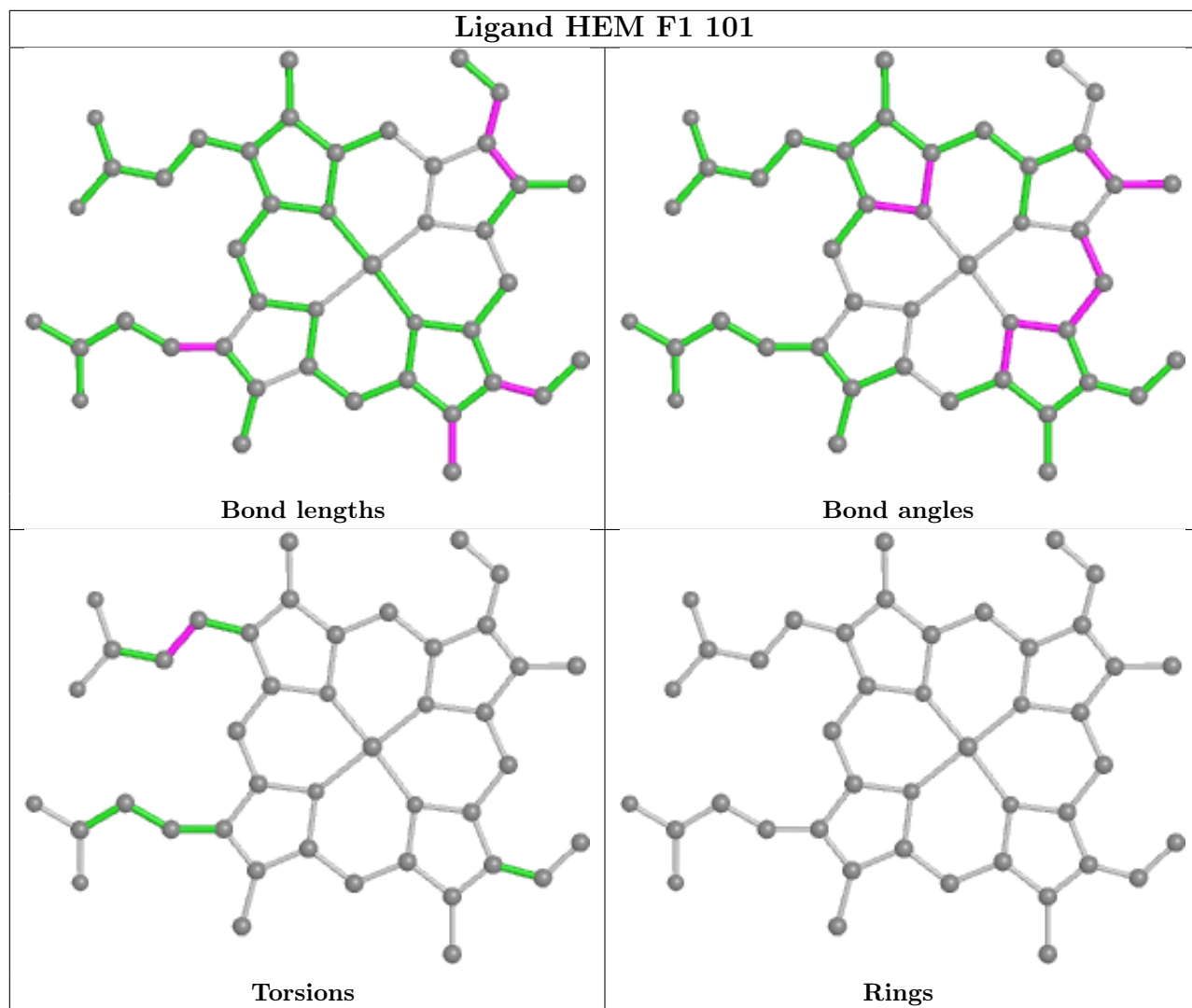
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

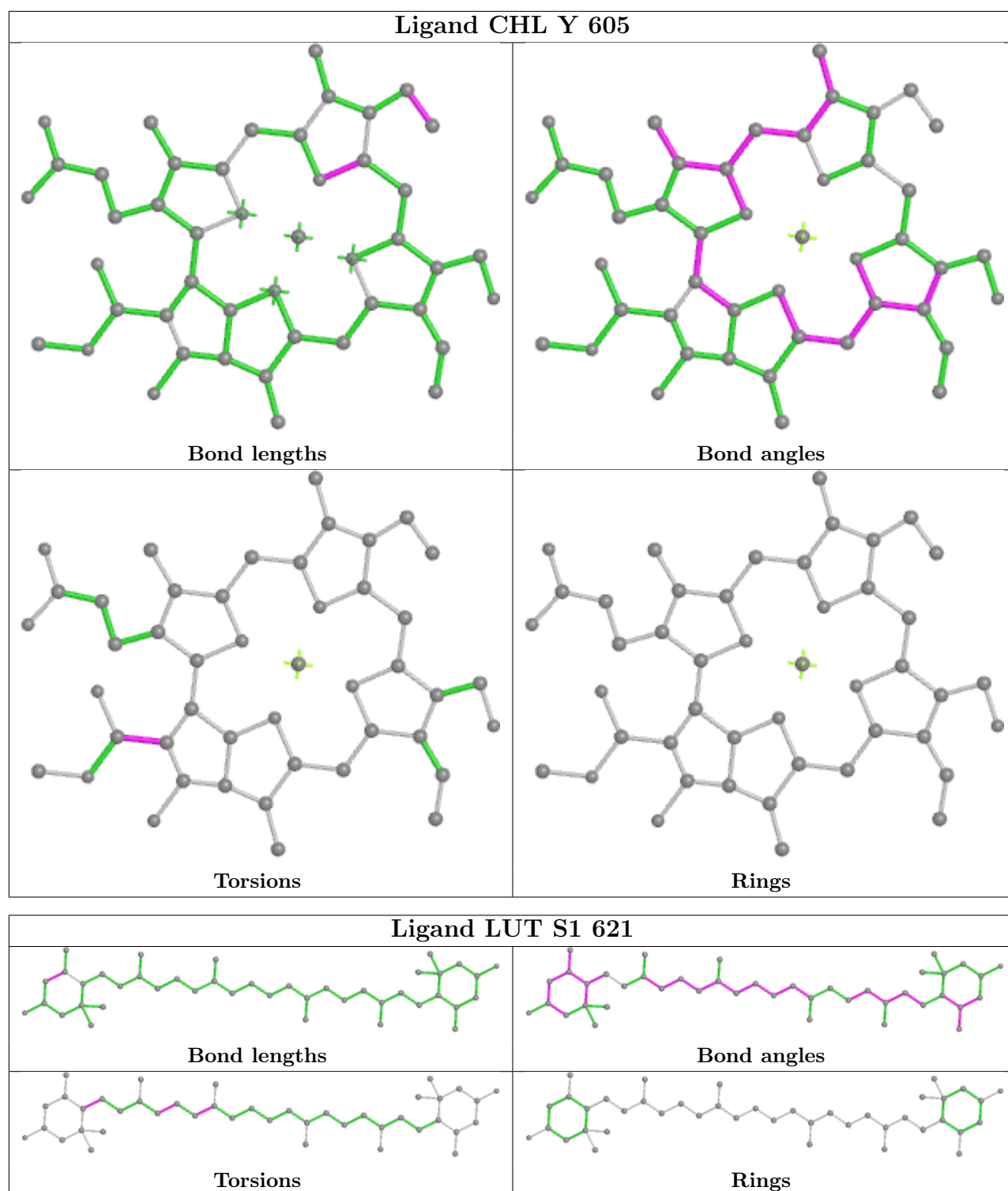
equivalents in the CSD to analyse the geometry.



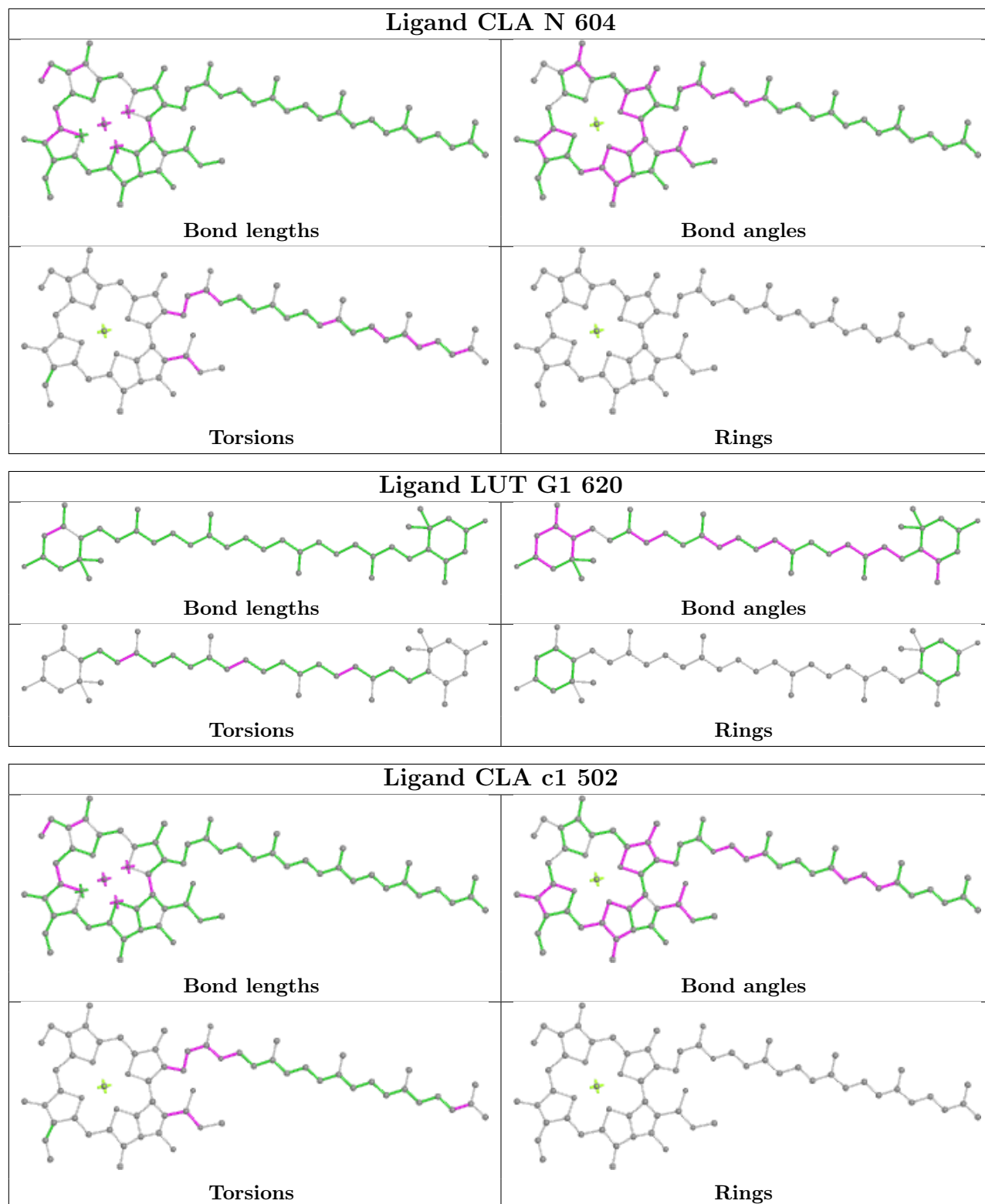


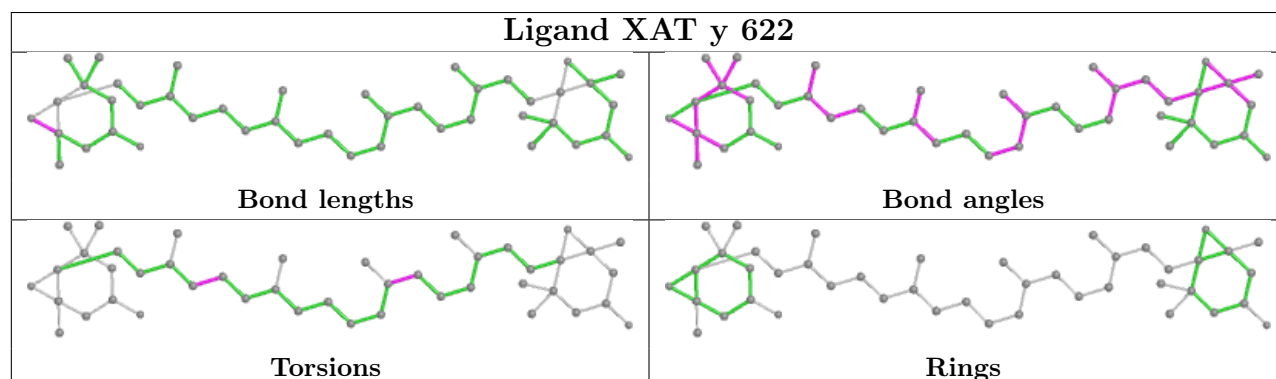
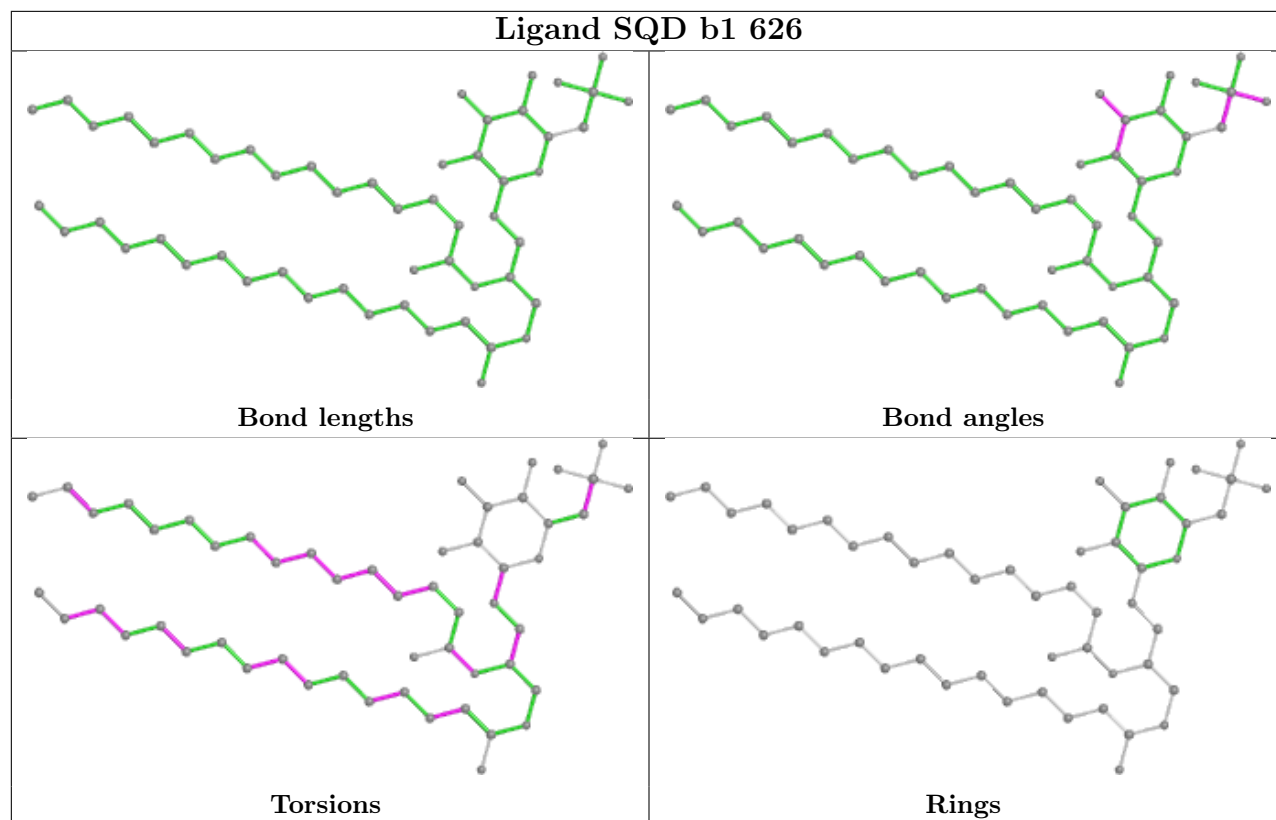


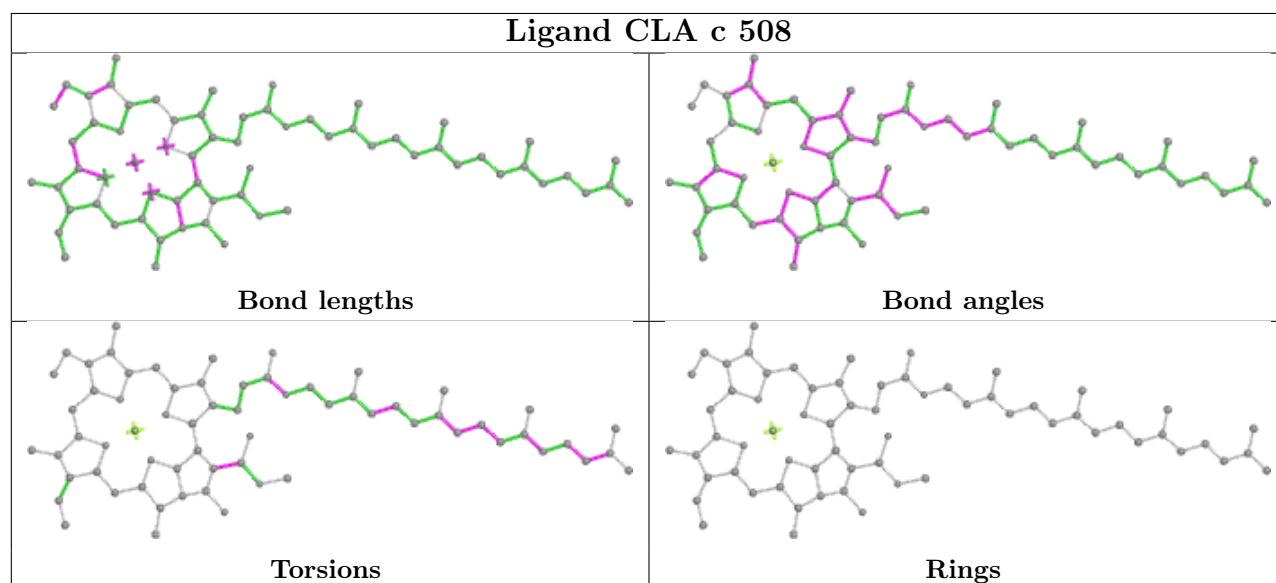
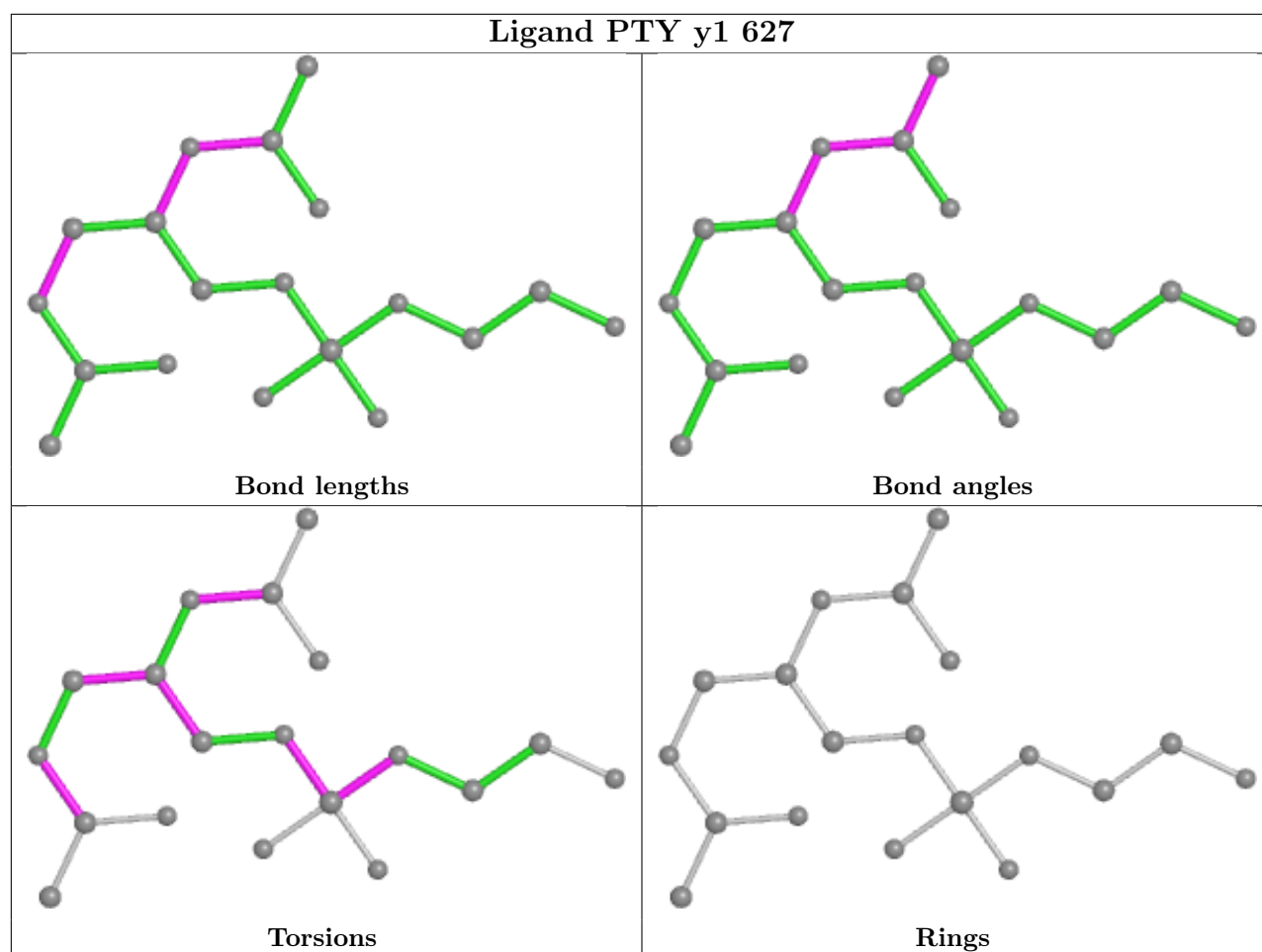


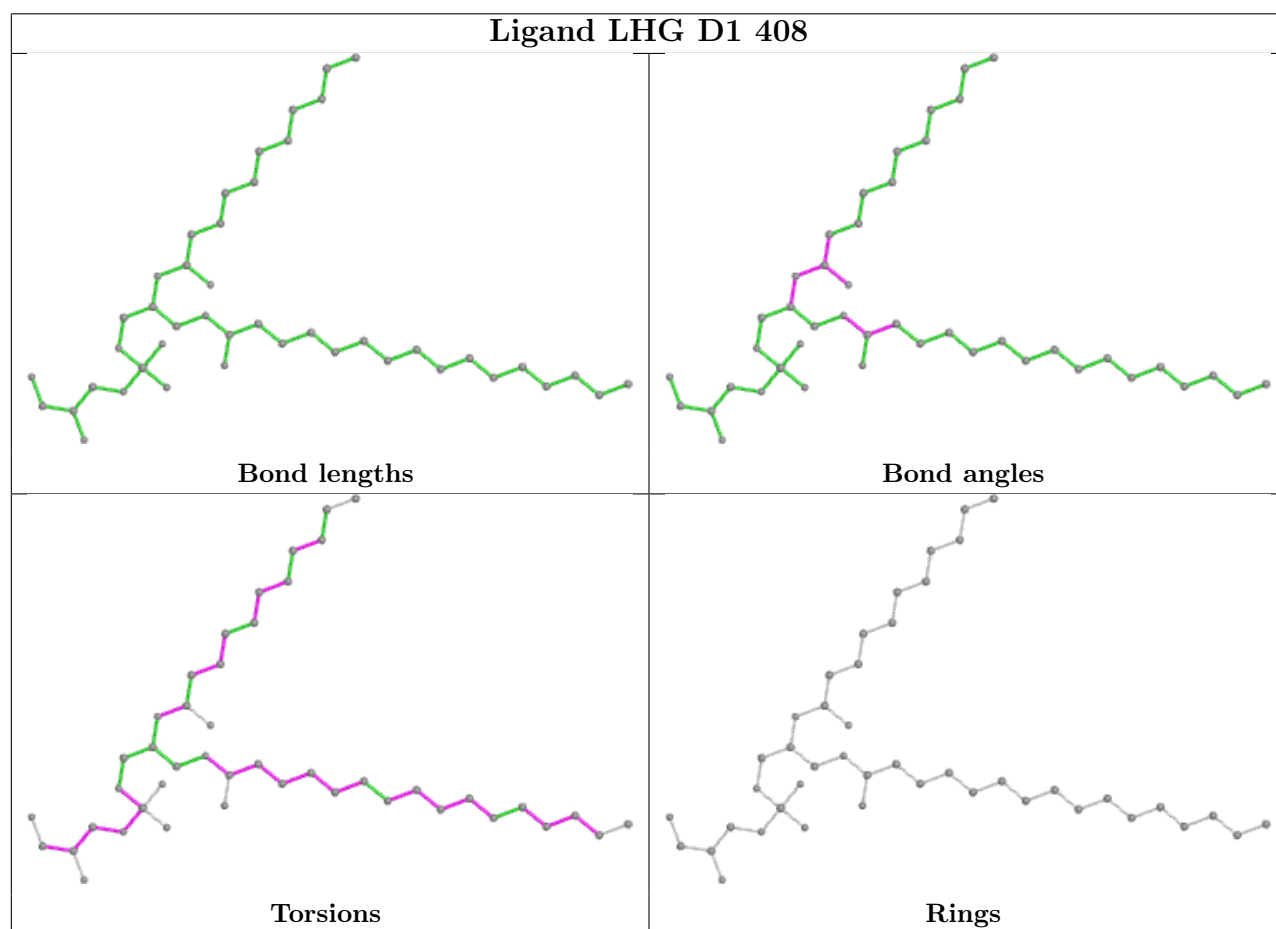
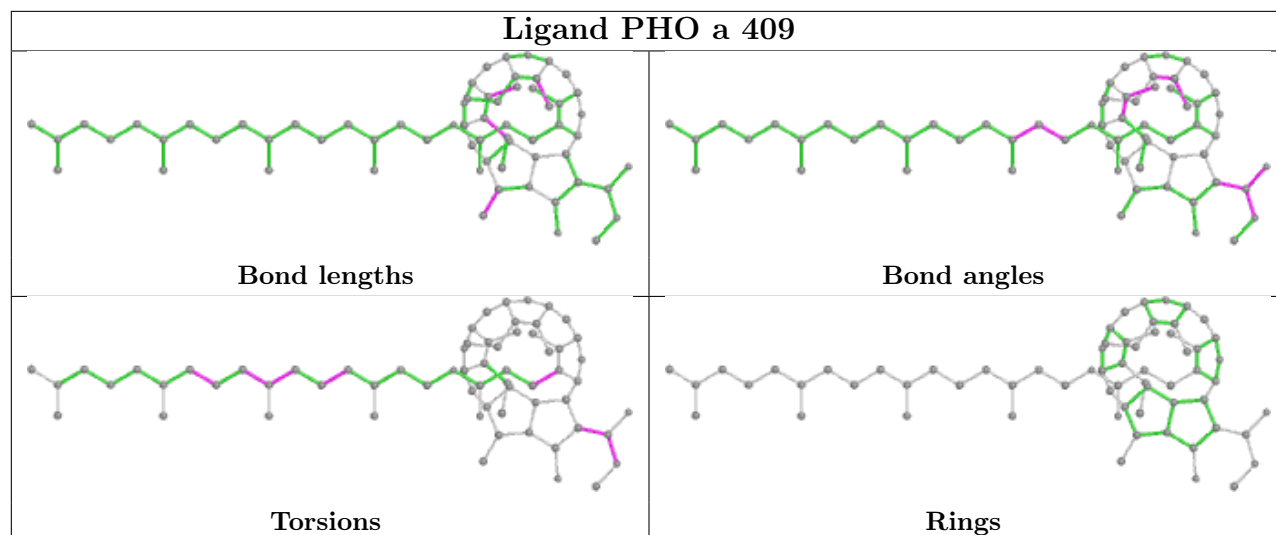


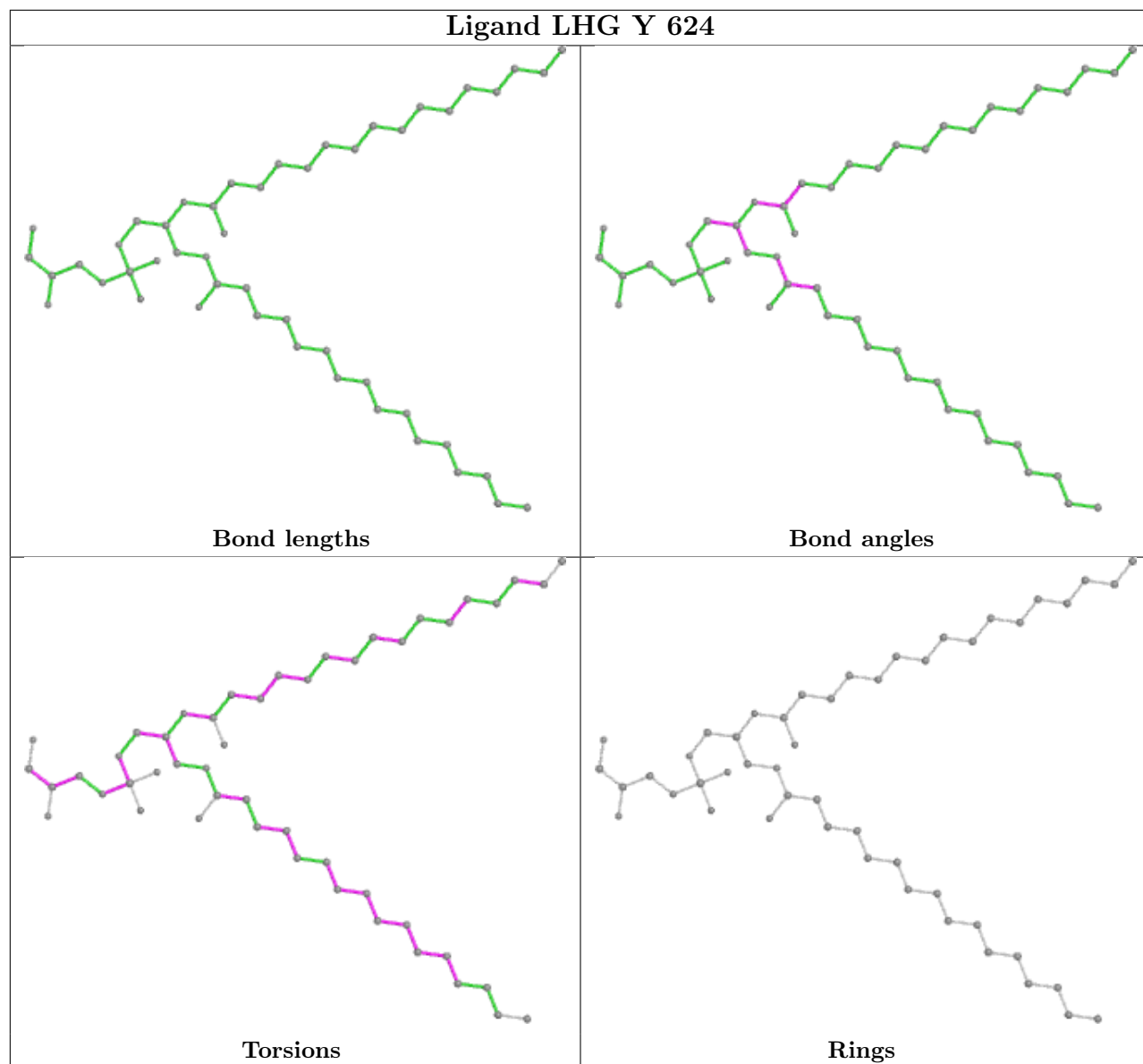


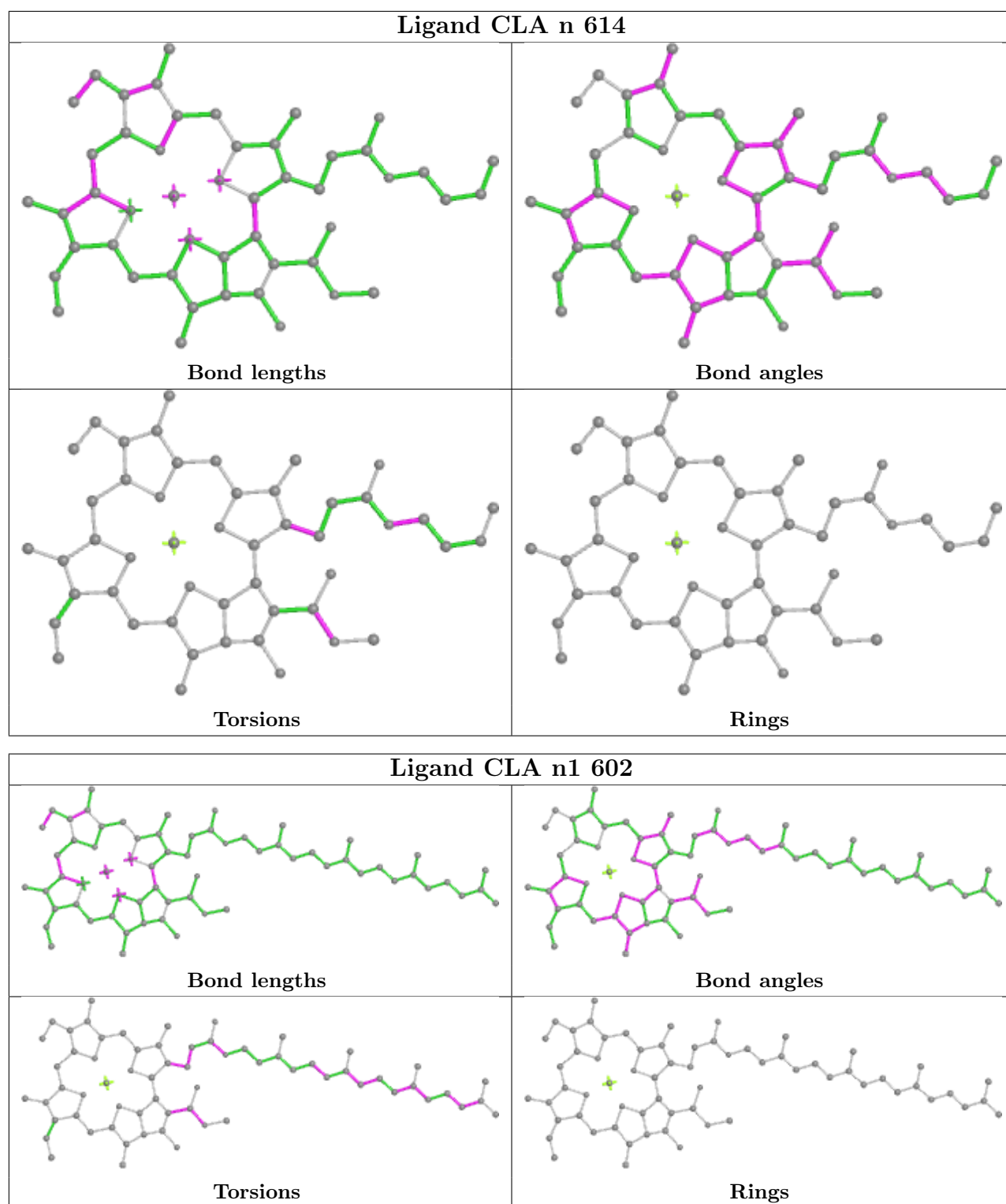


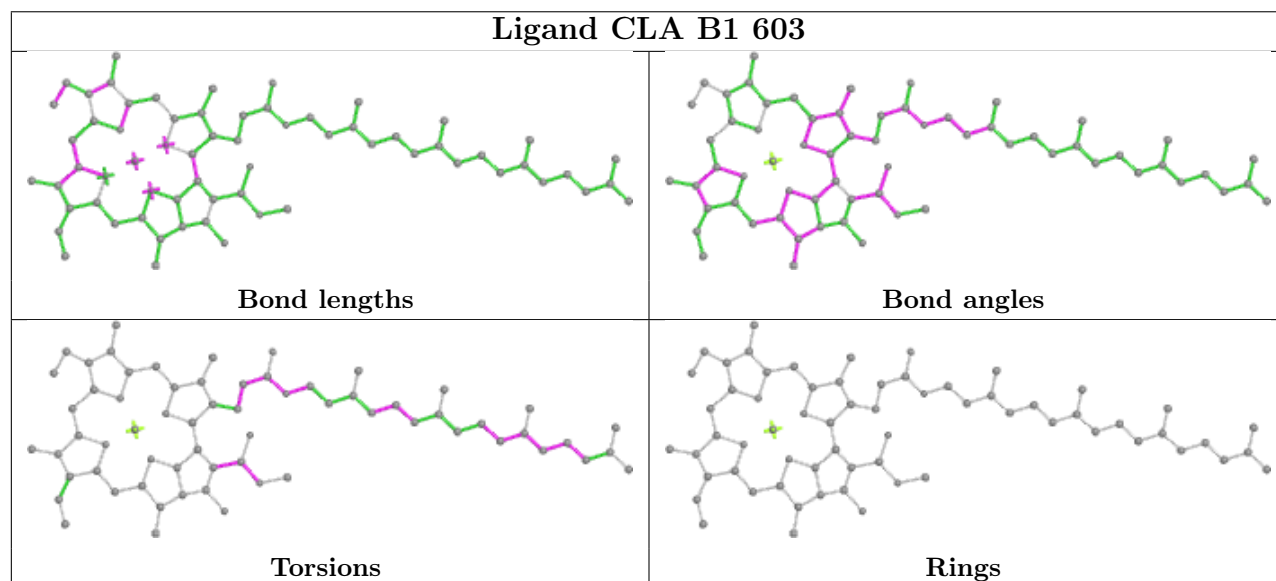
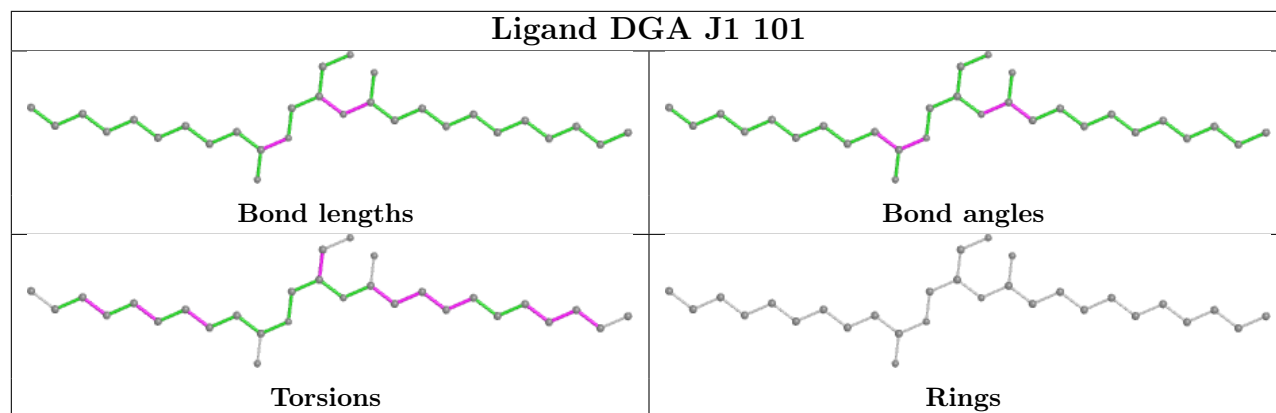


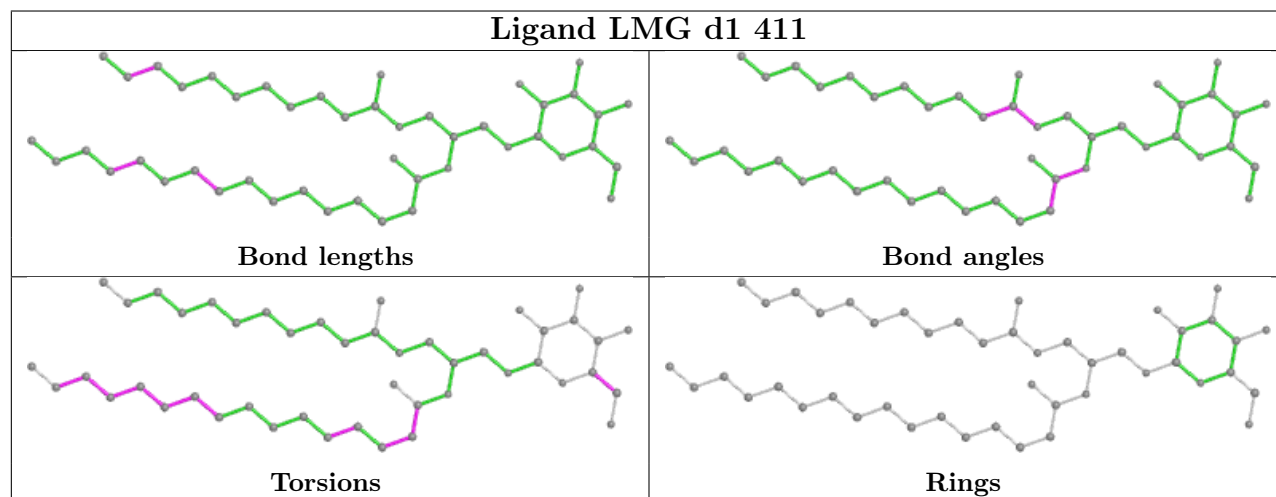
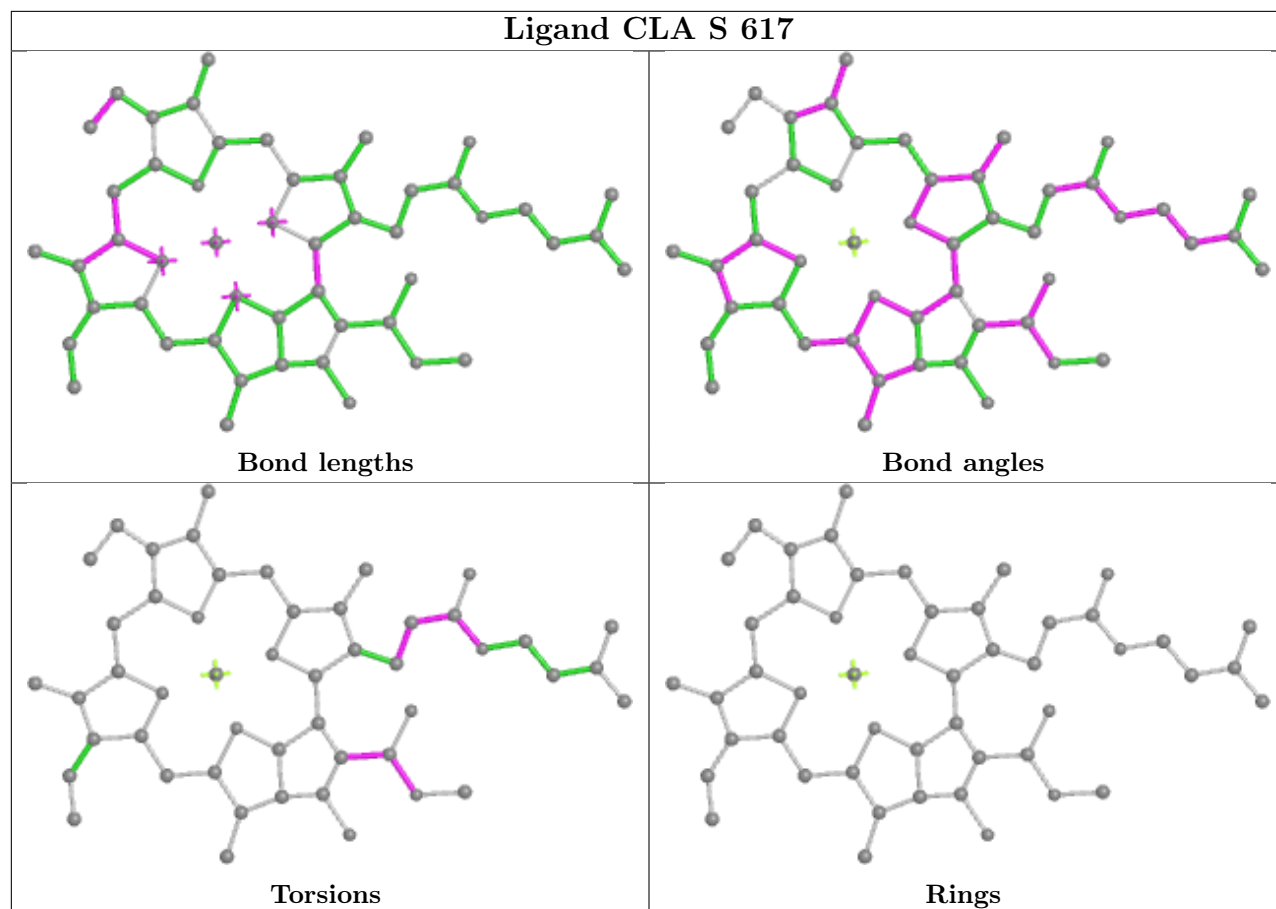




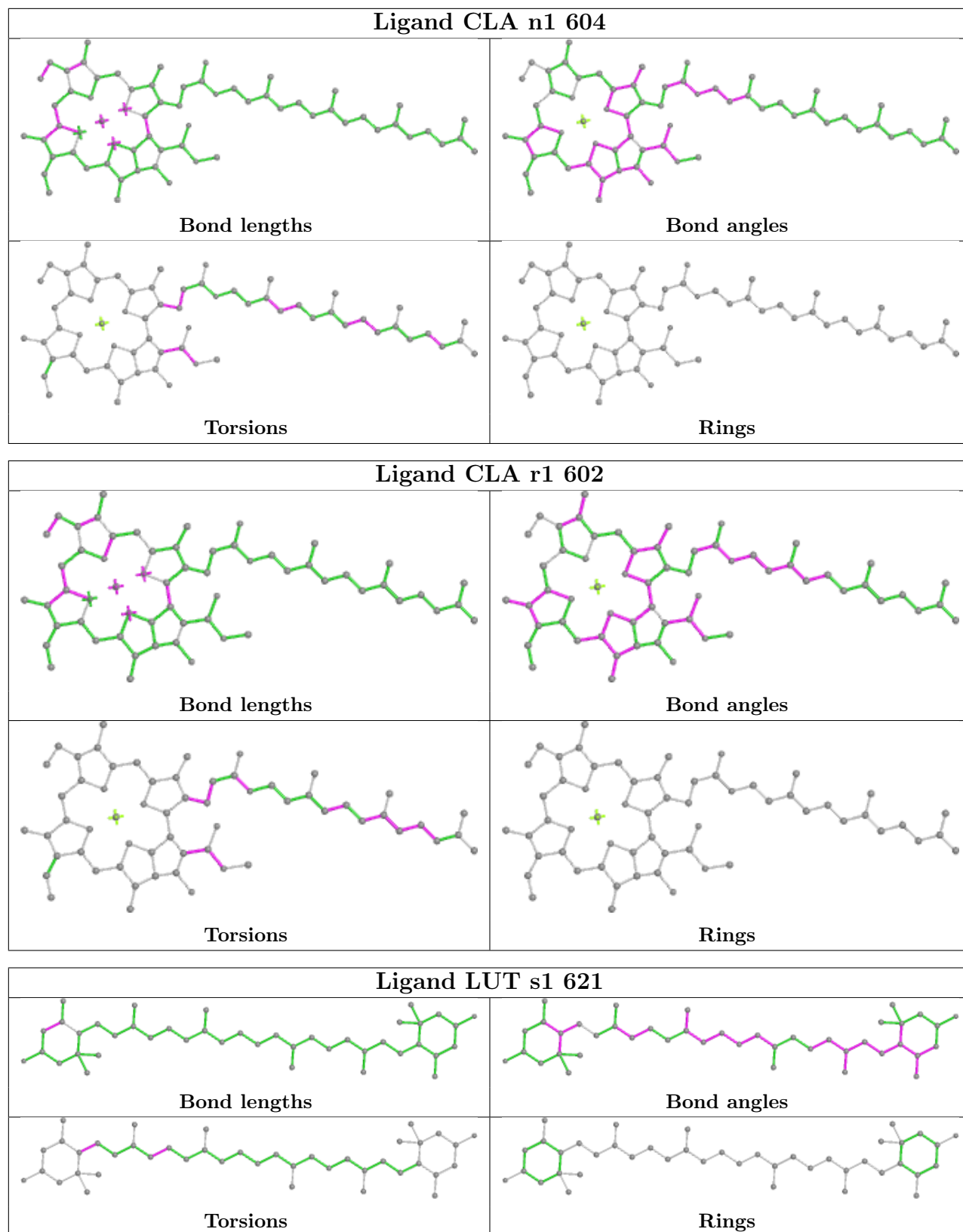


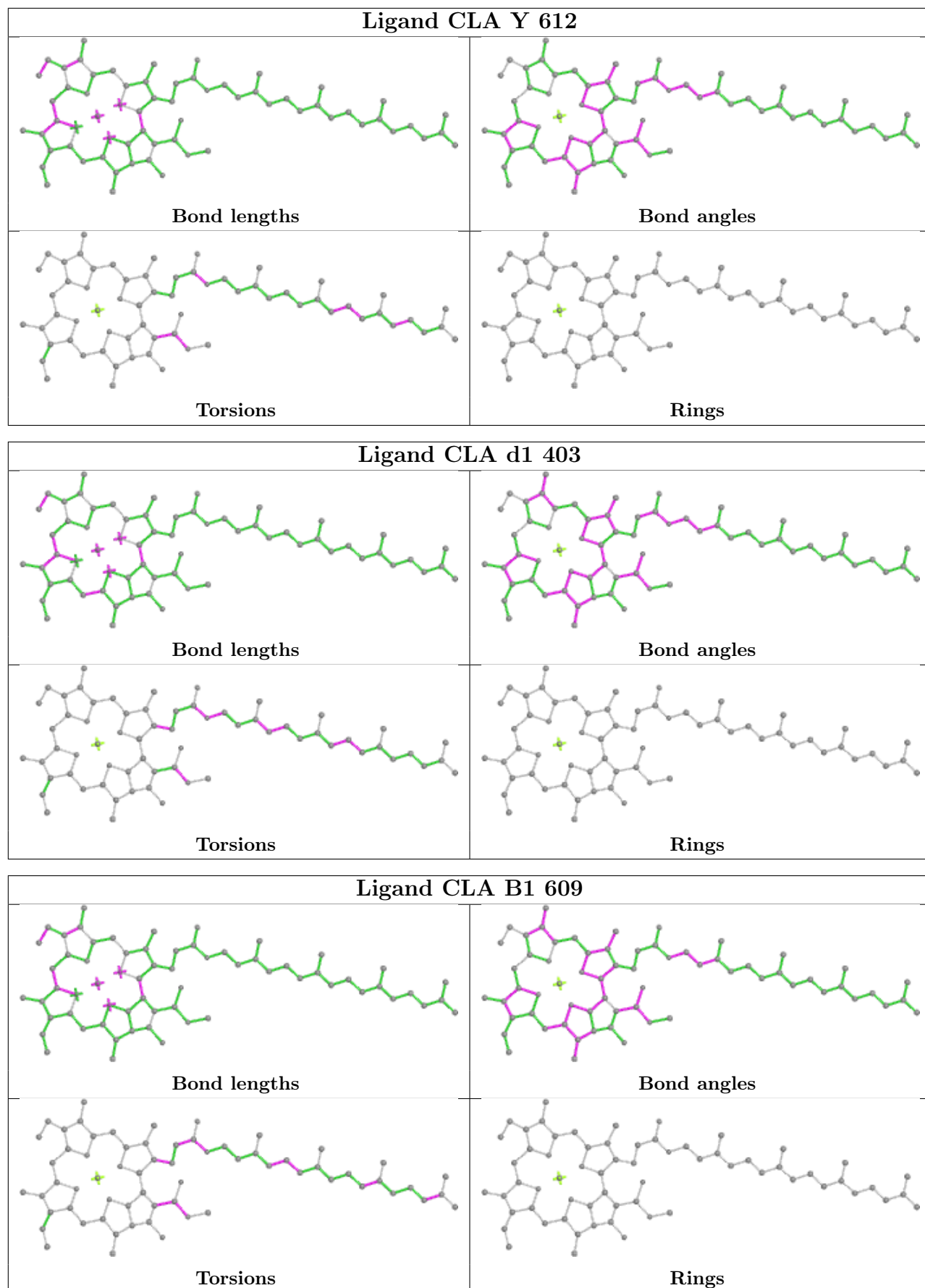


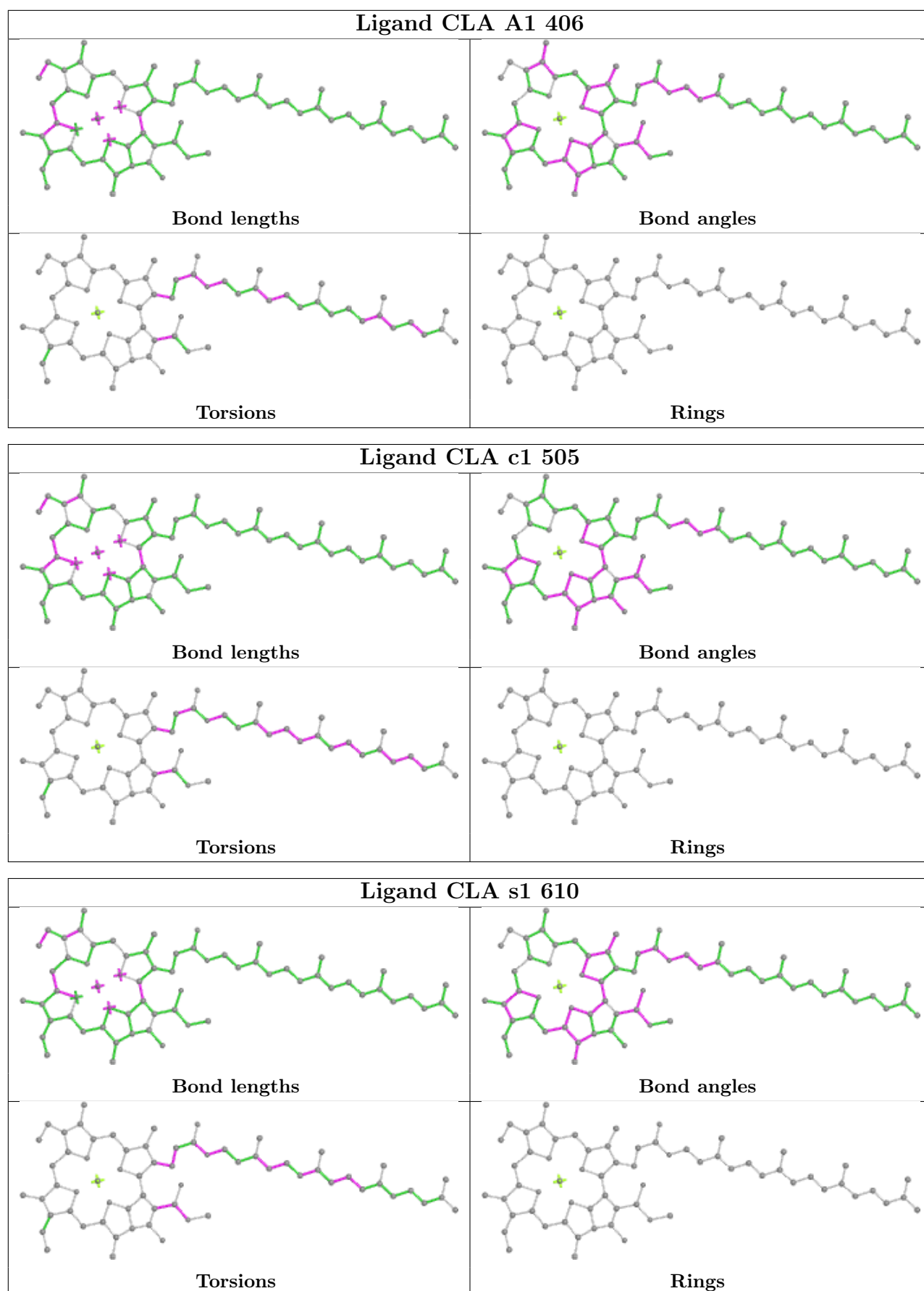


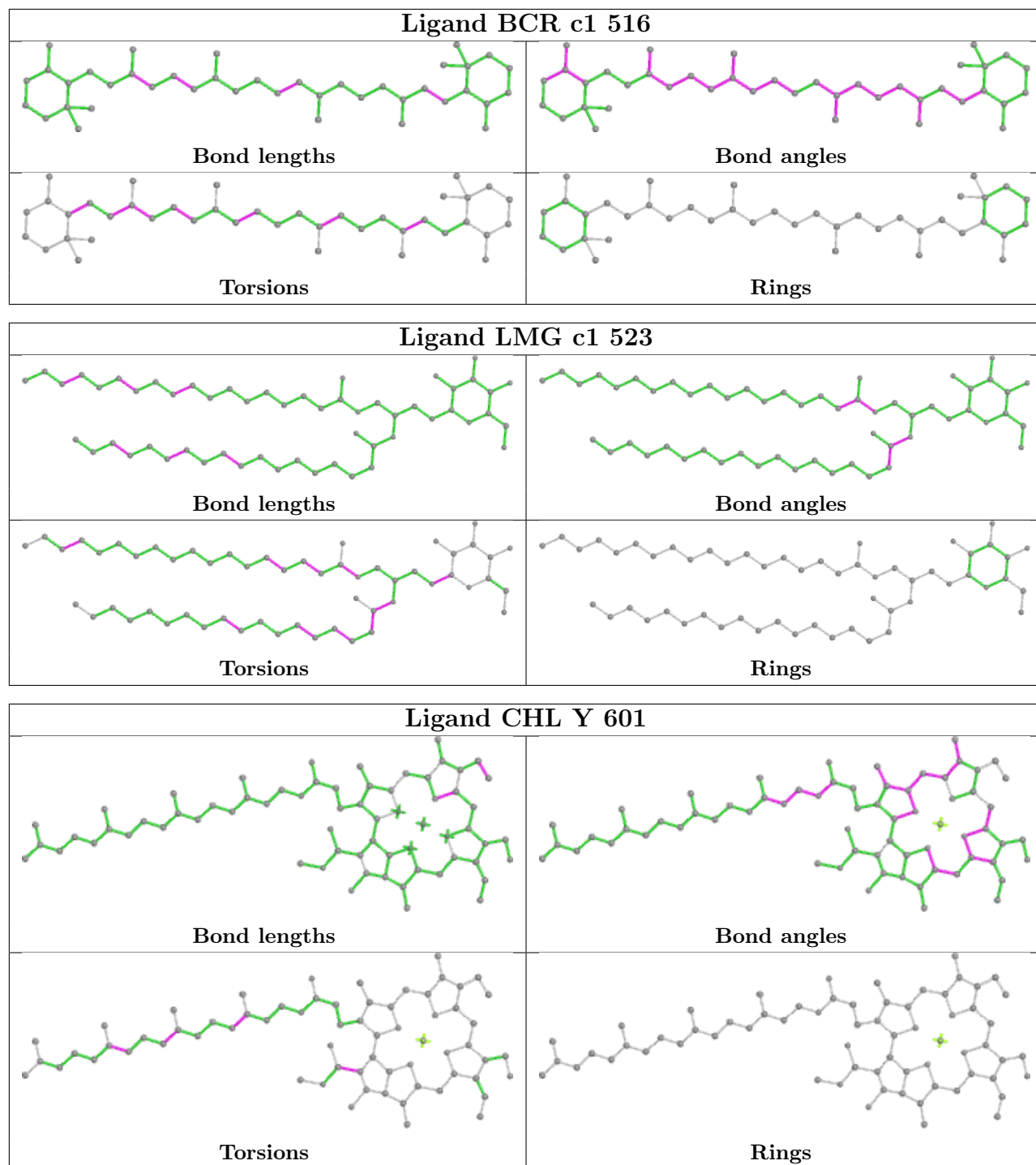


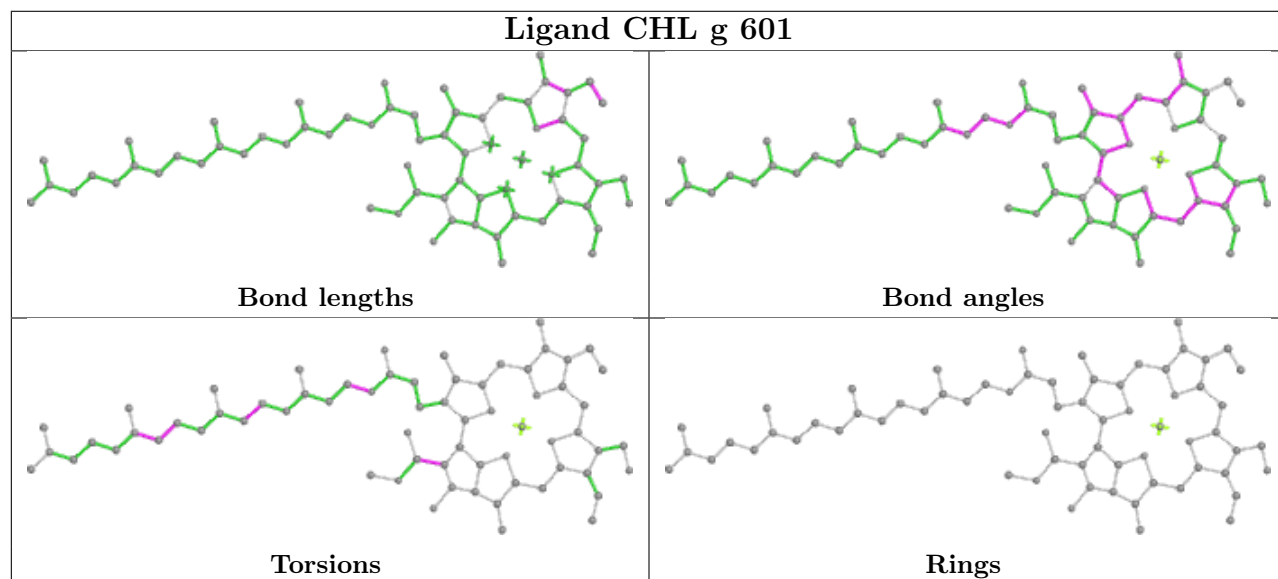
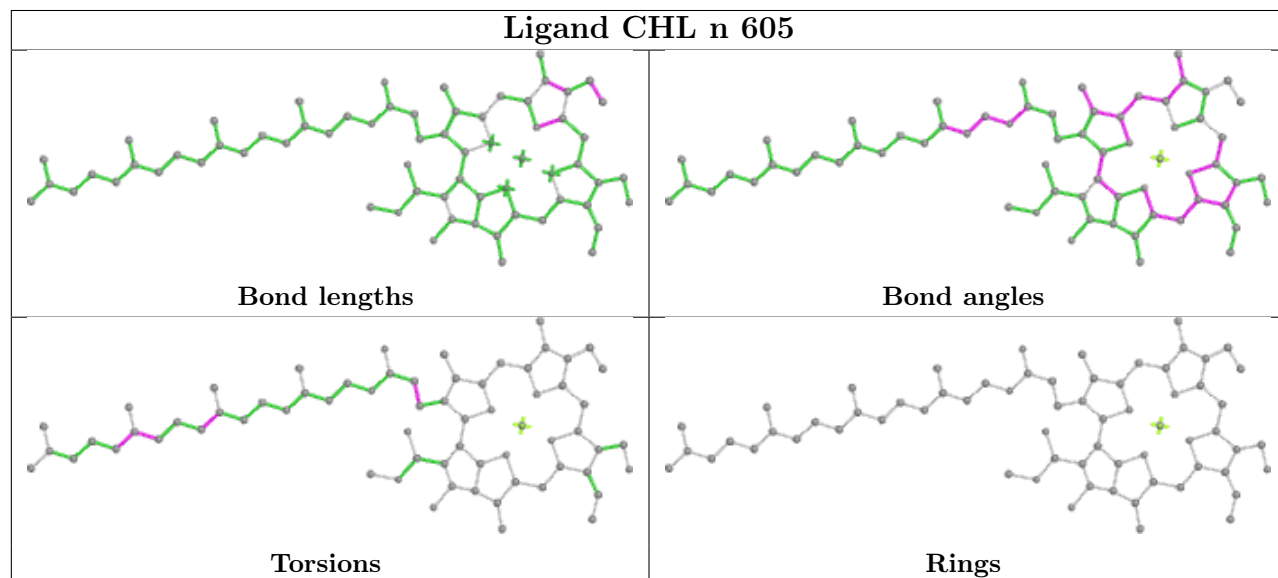
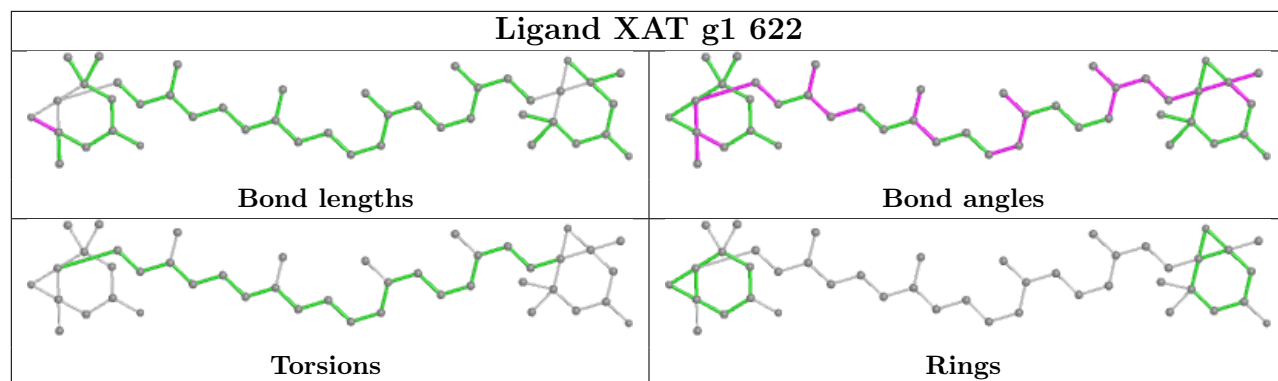


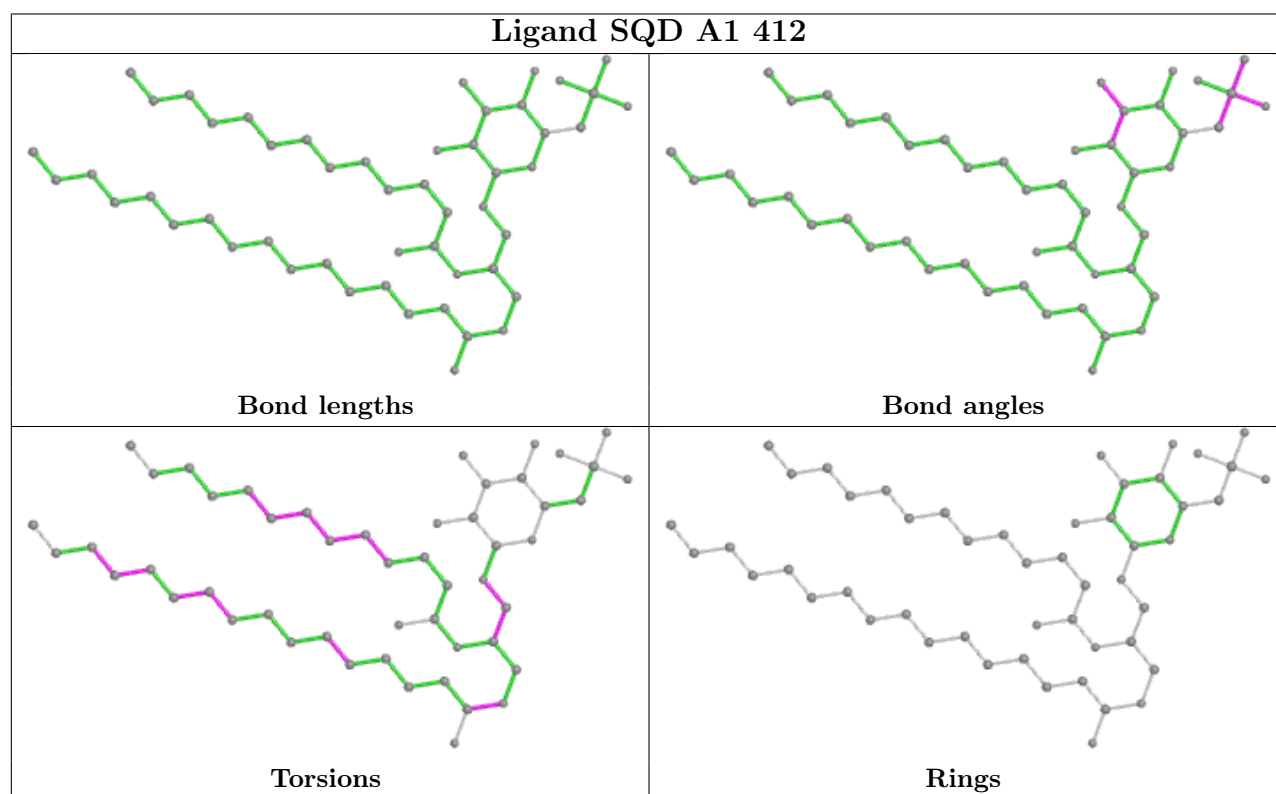
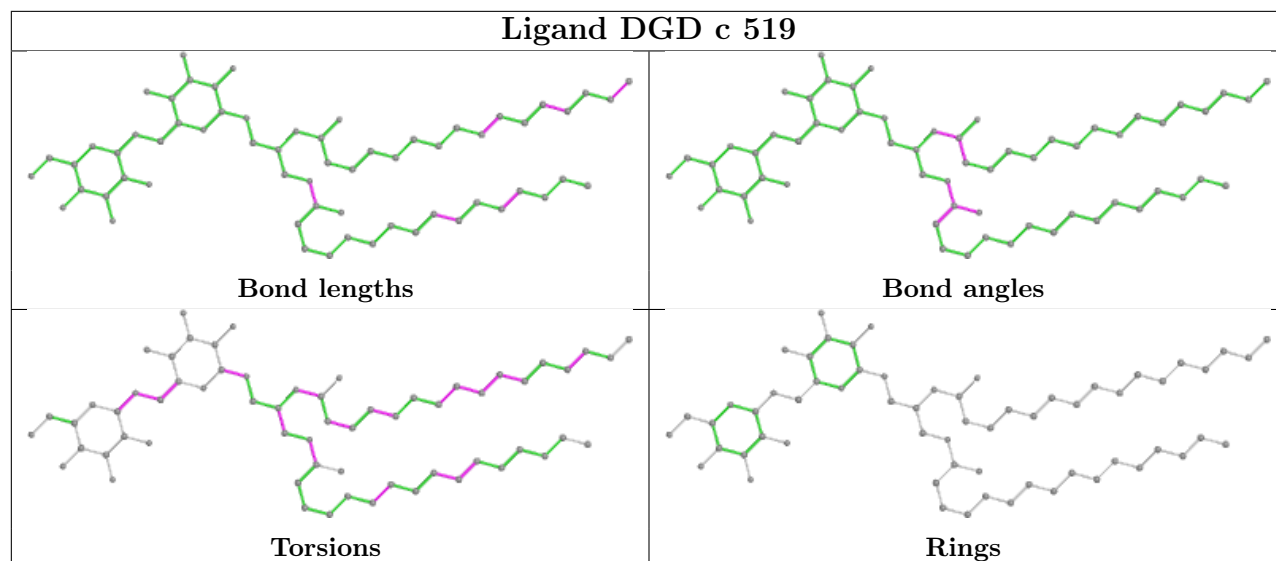


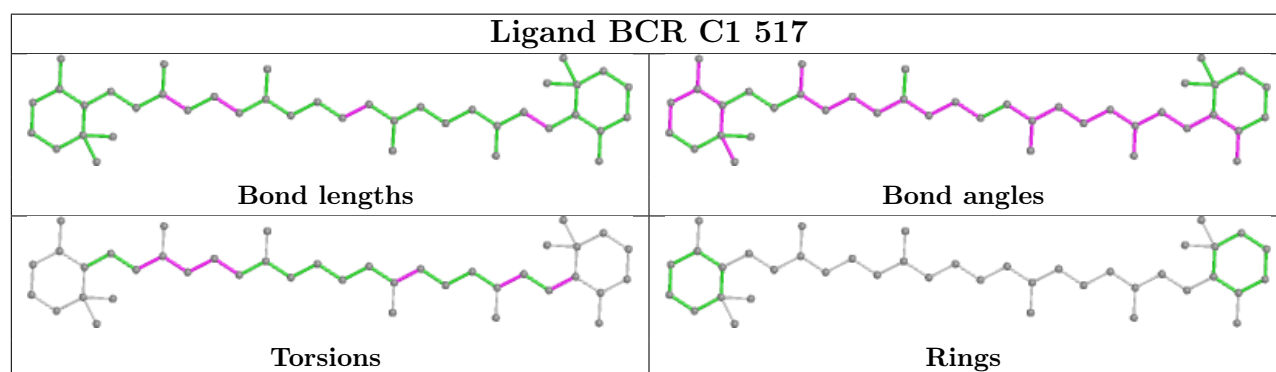
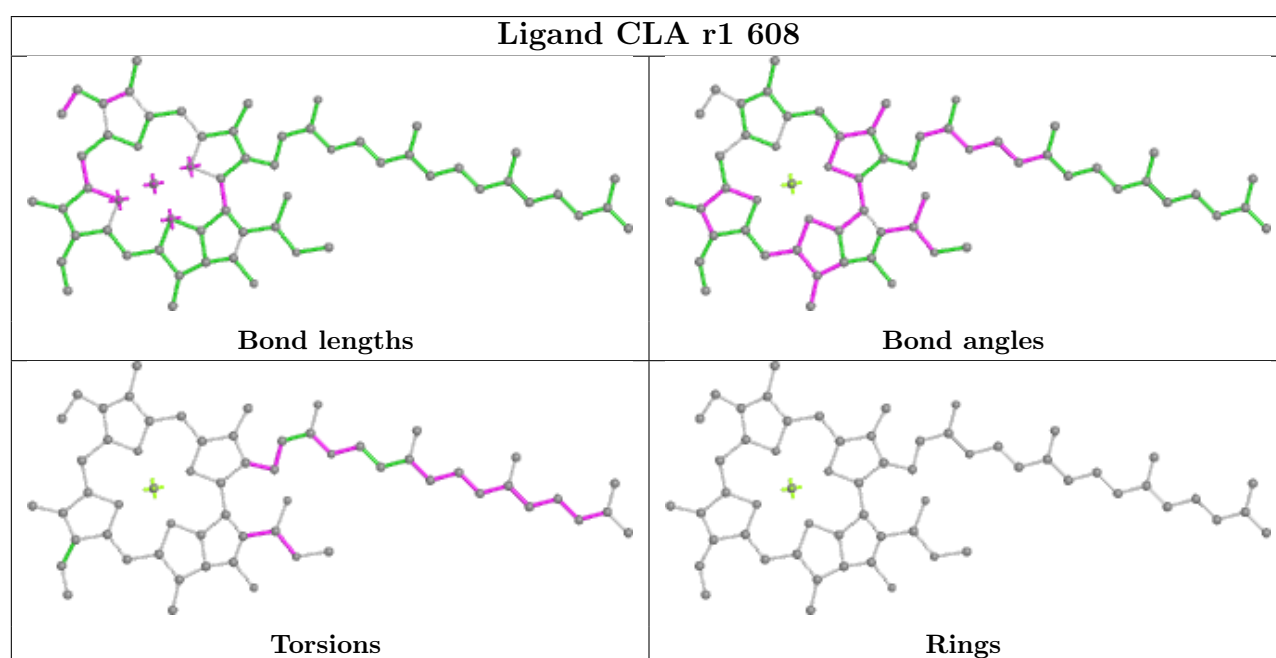
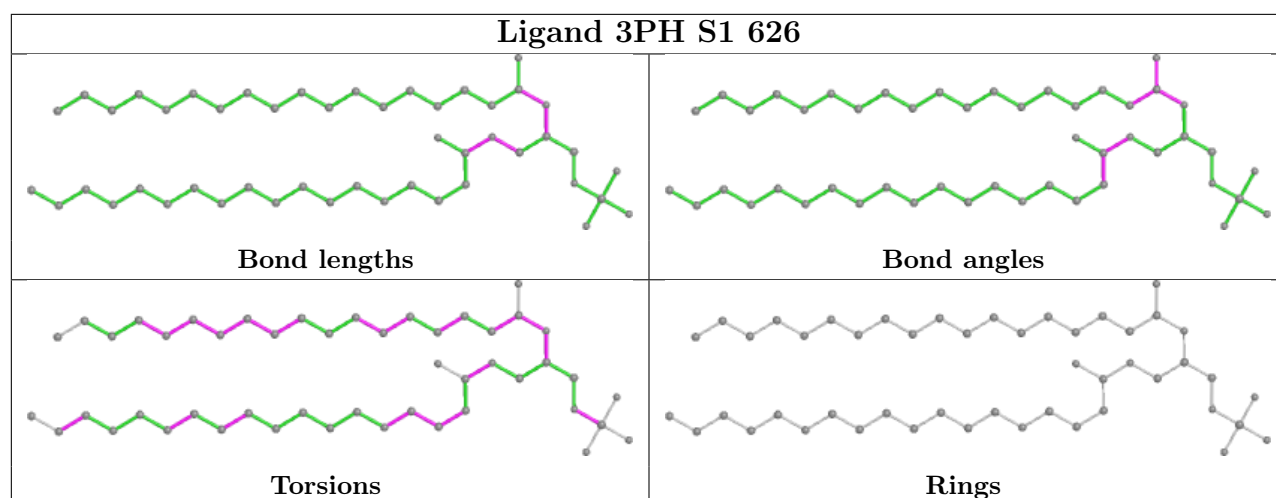


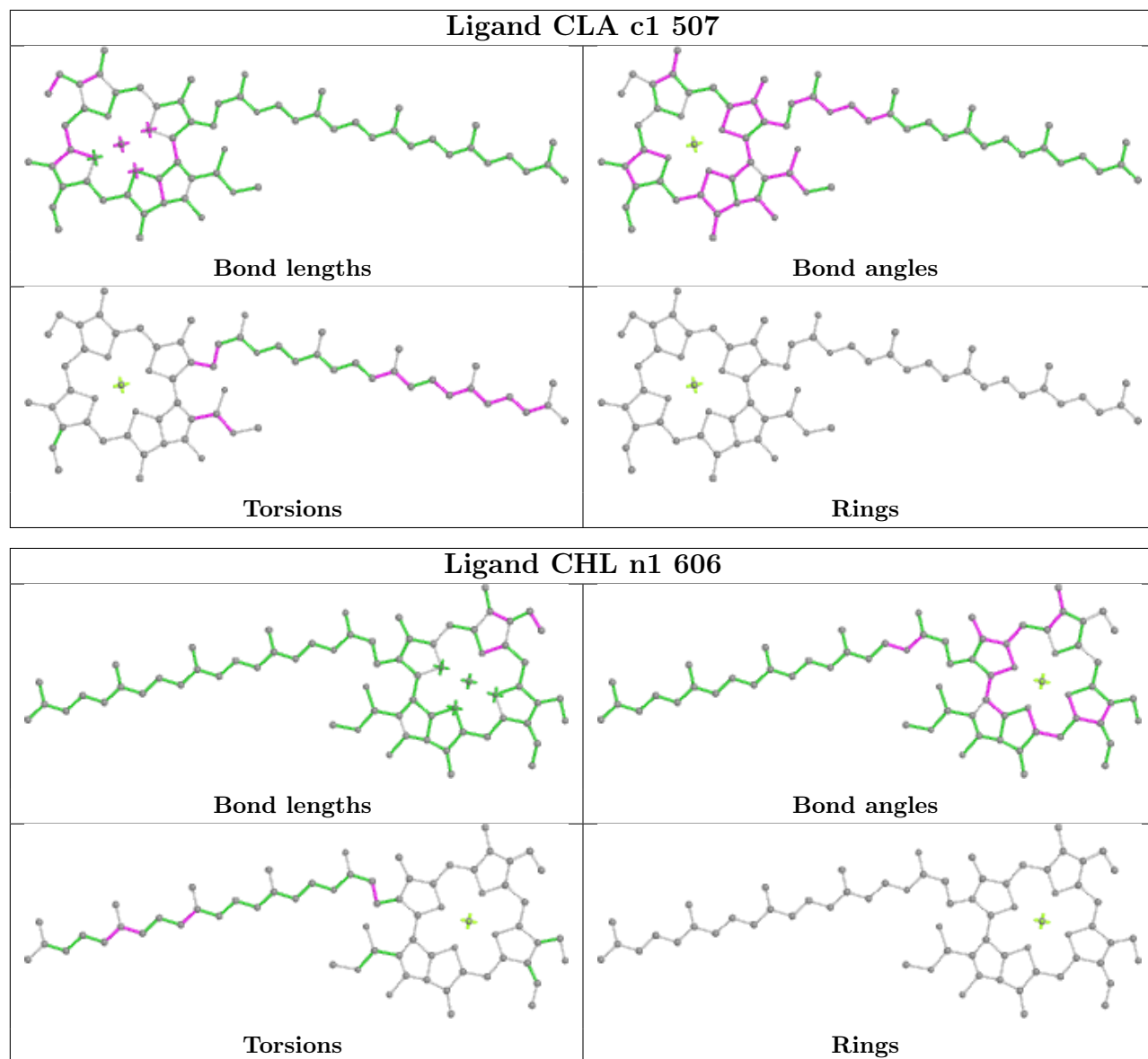




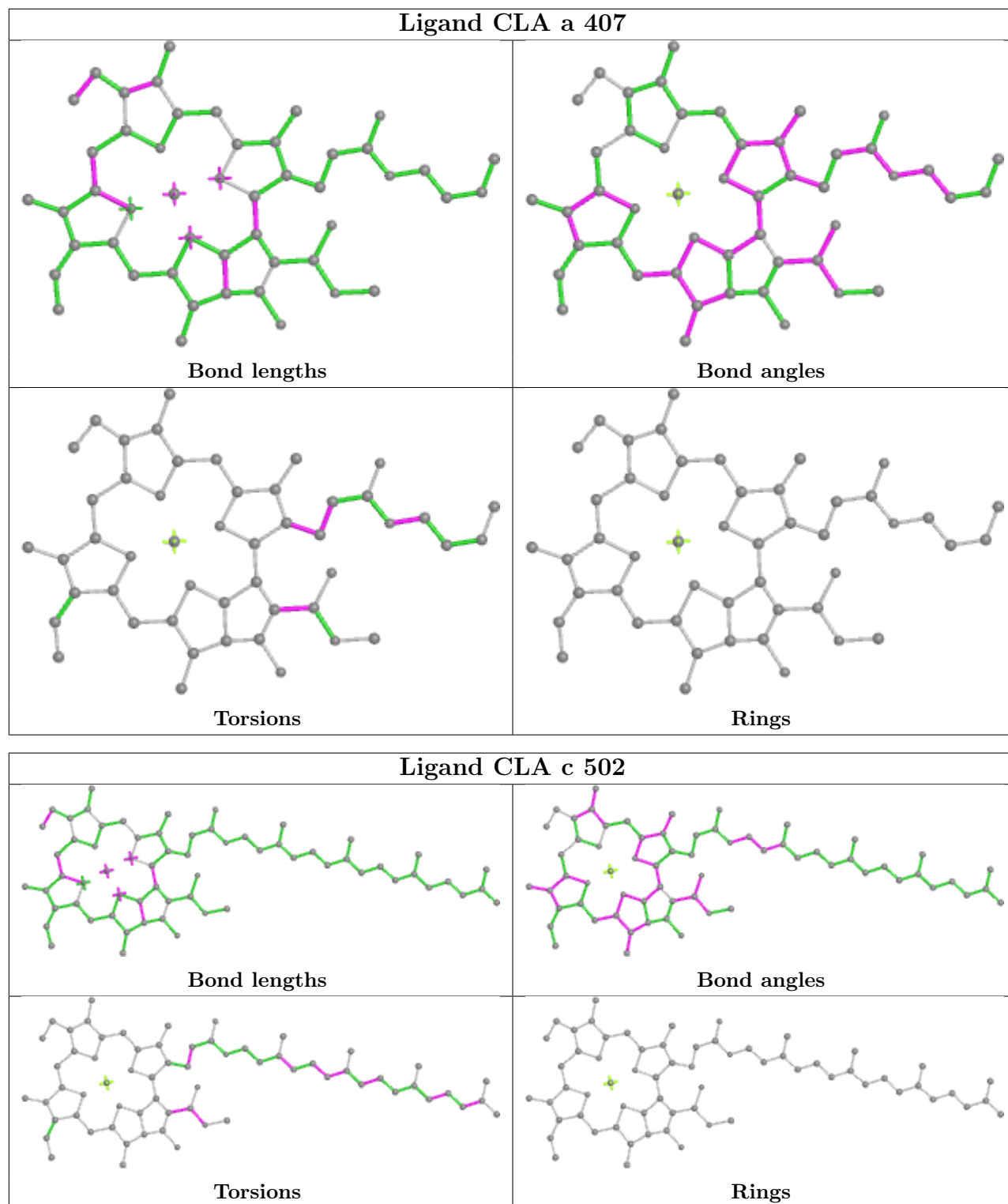


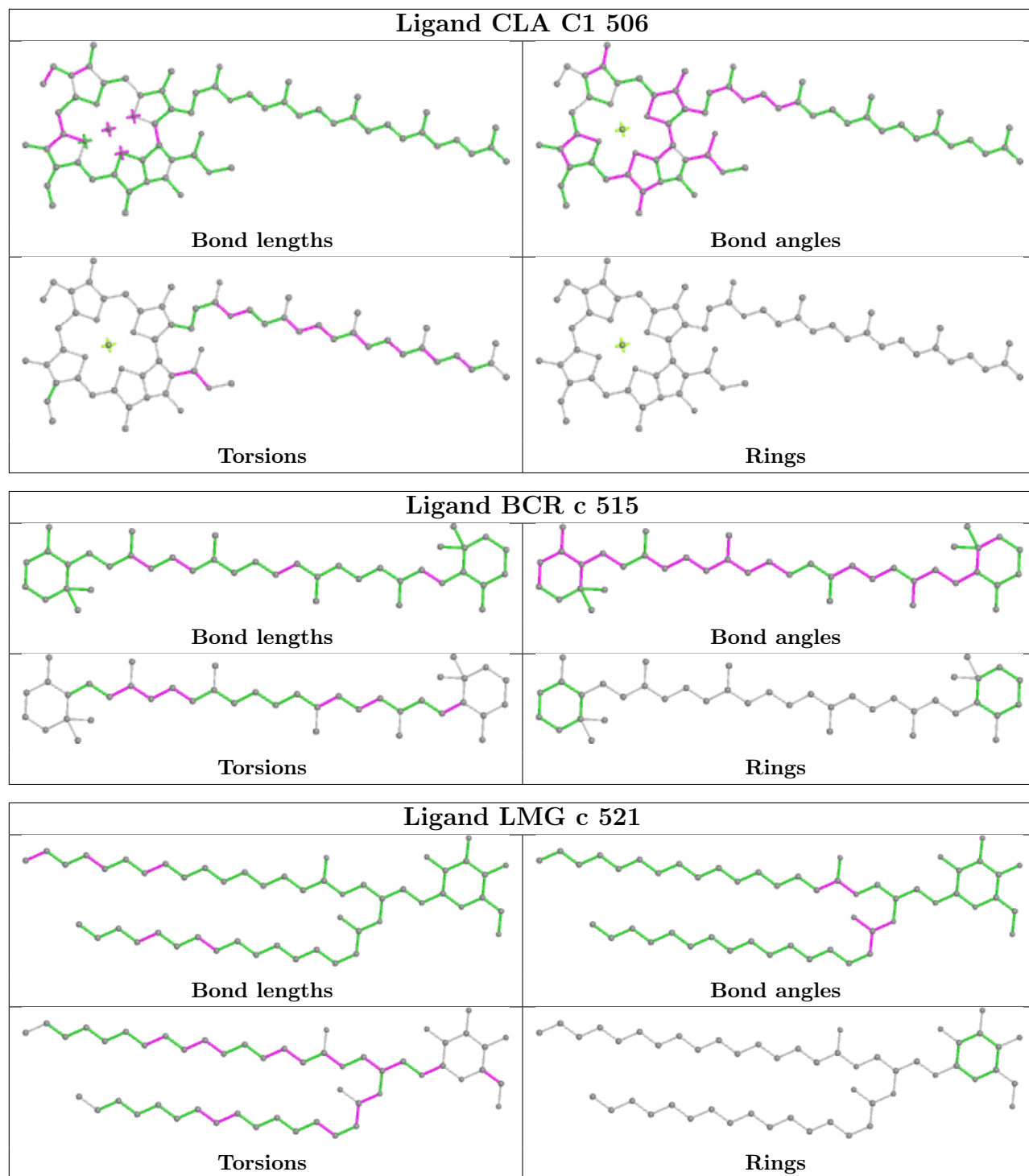


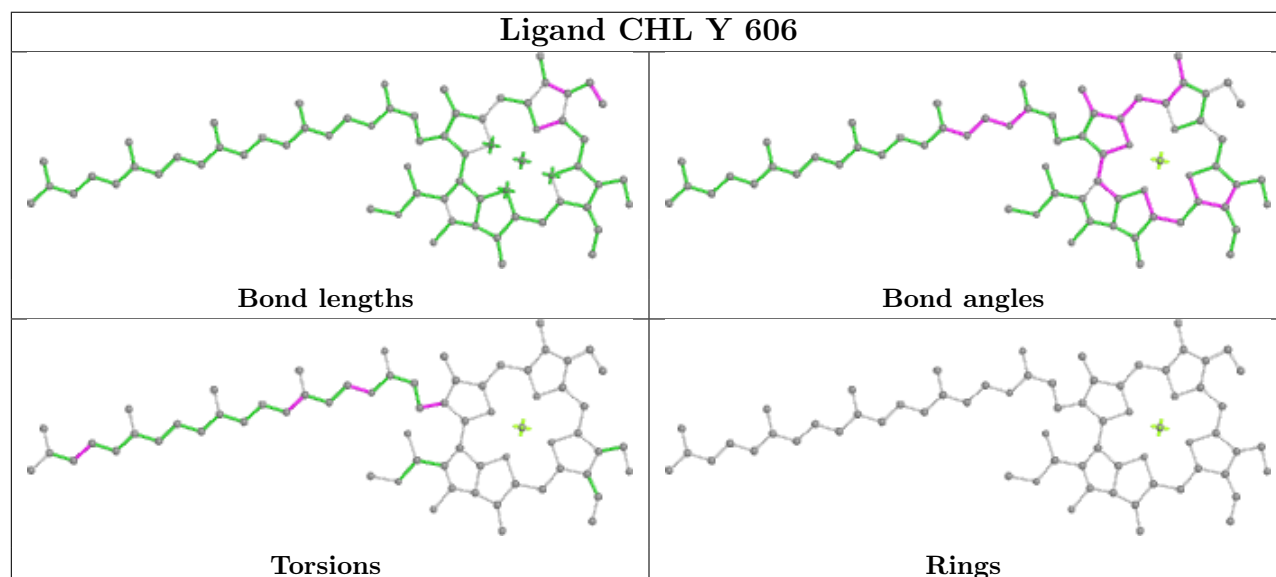
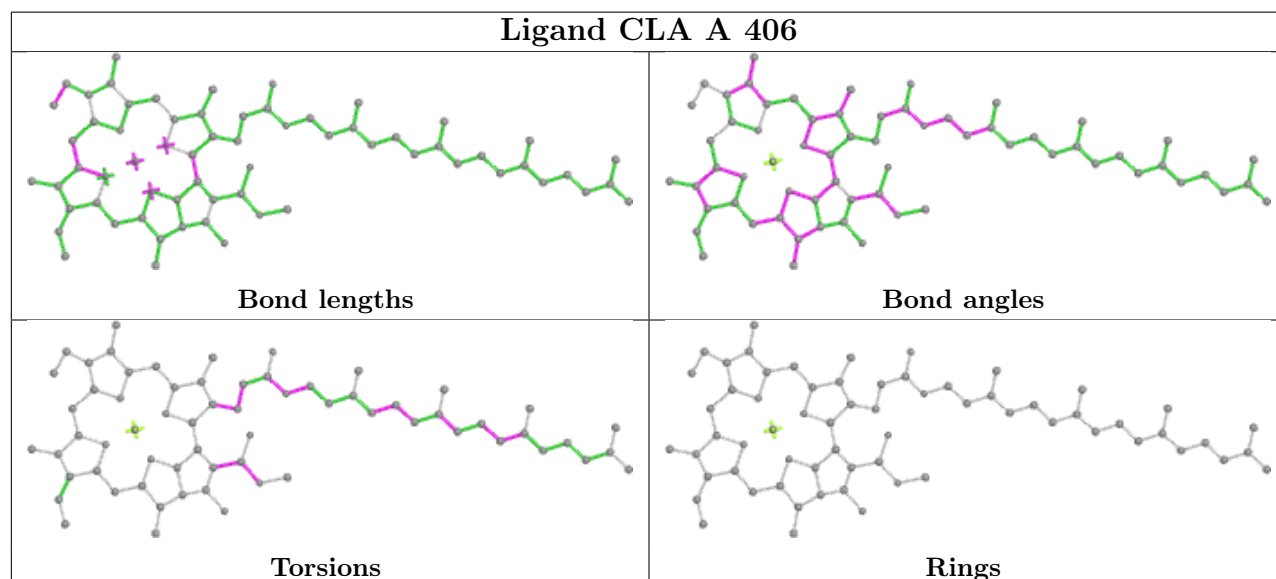
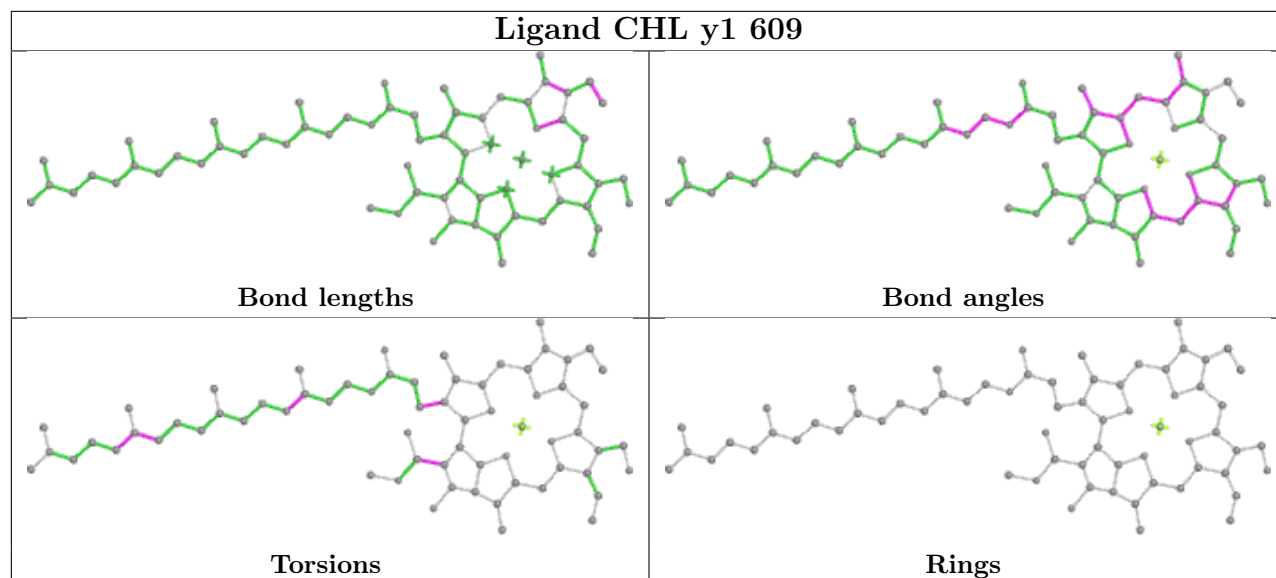


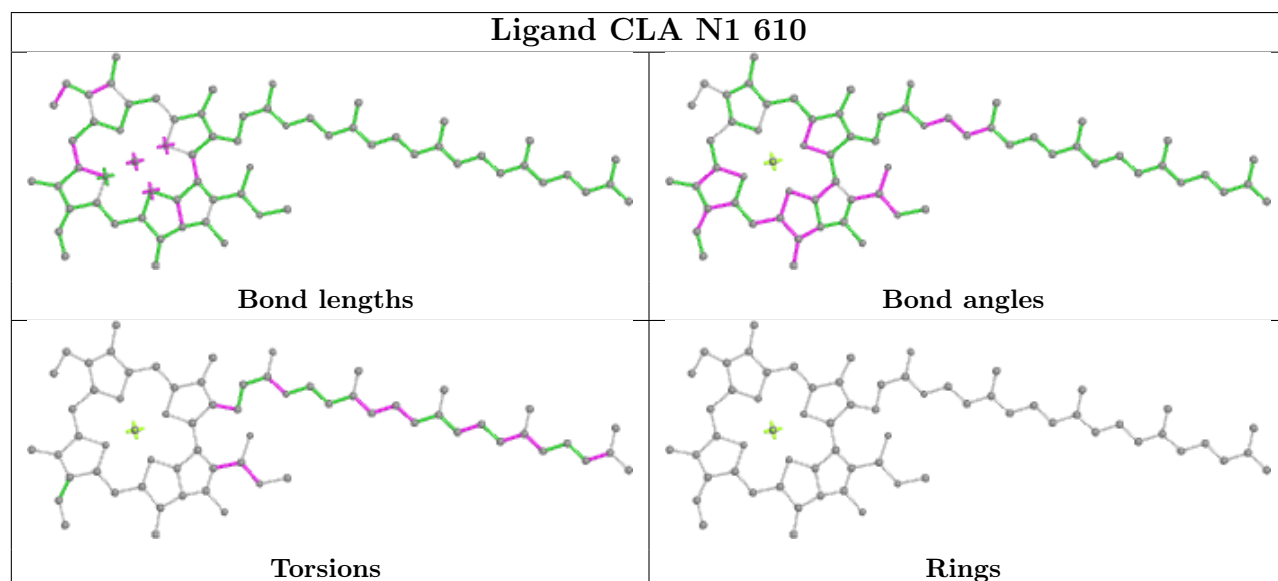
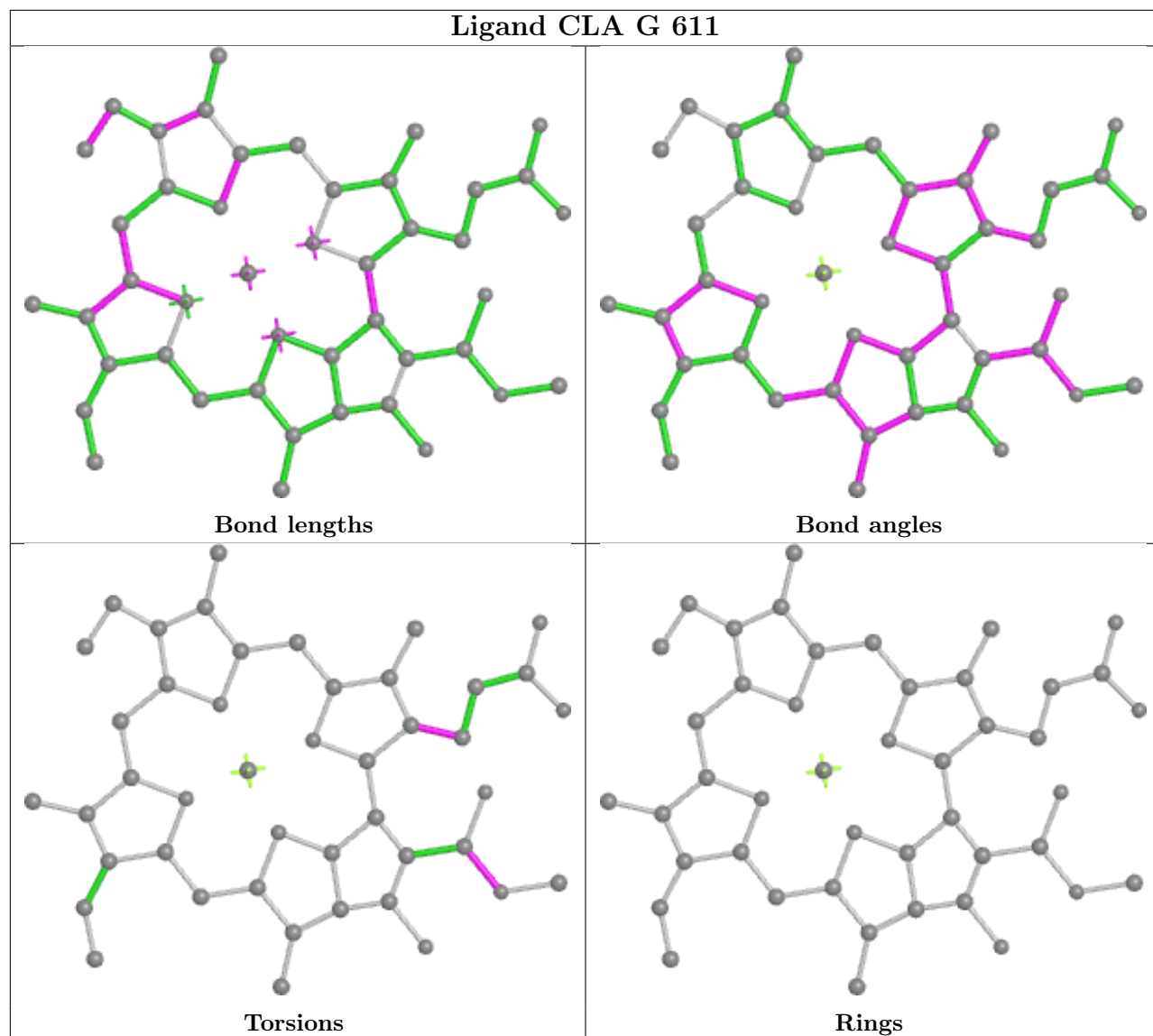


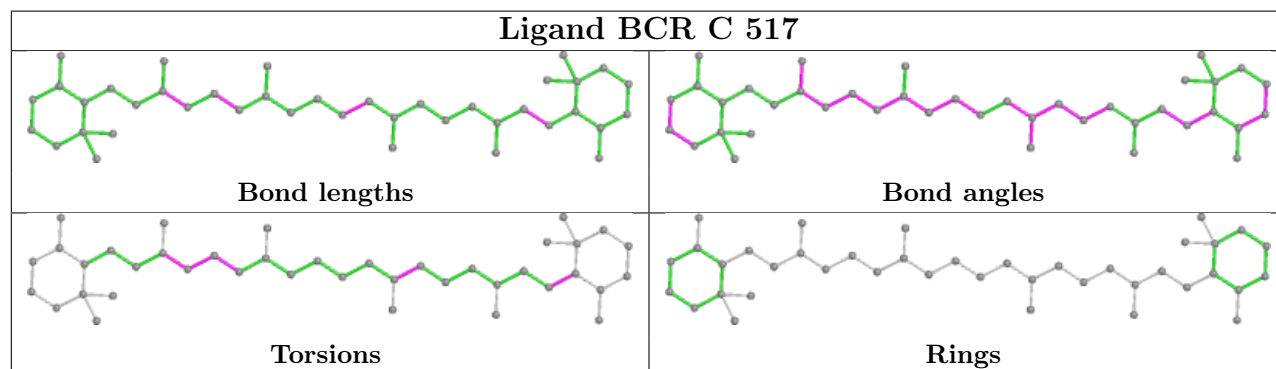
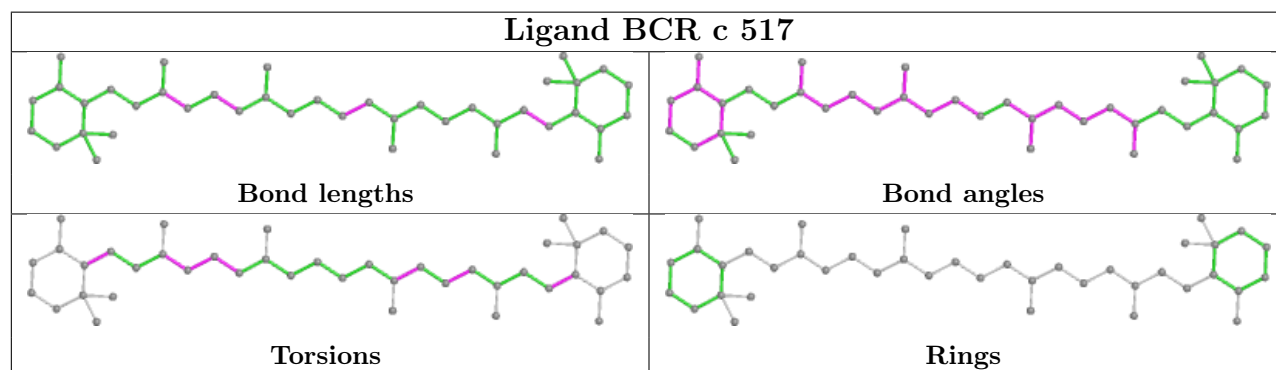
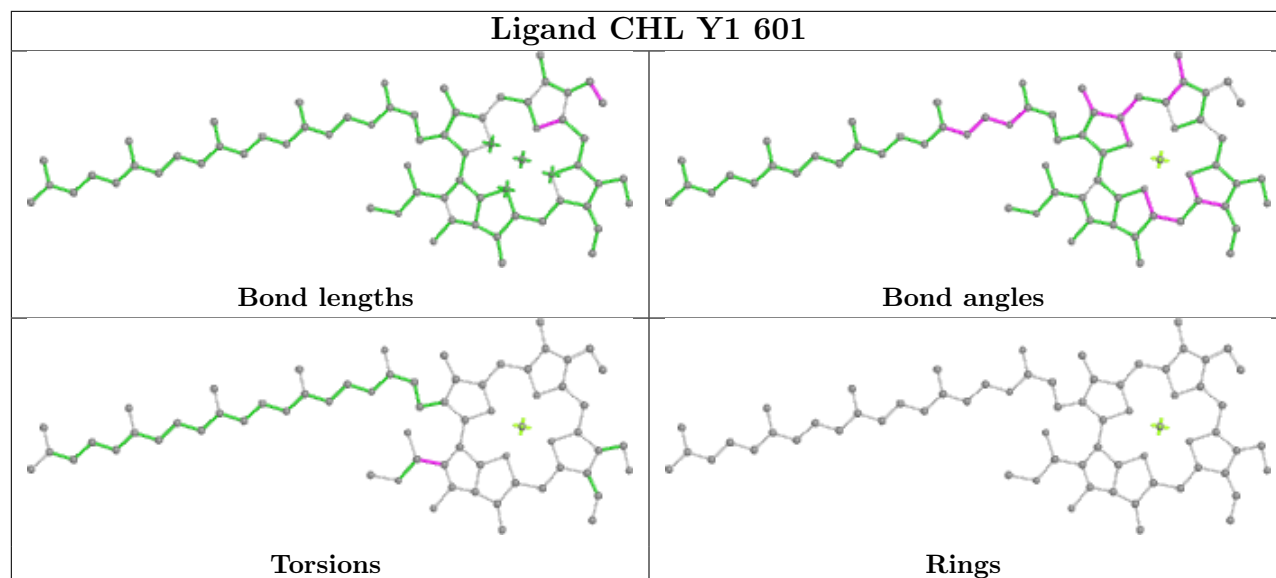


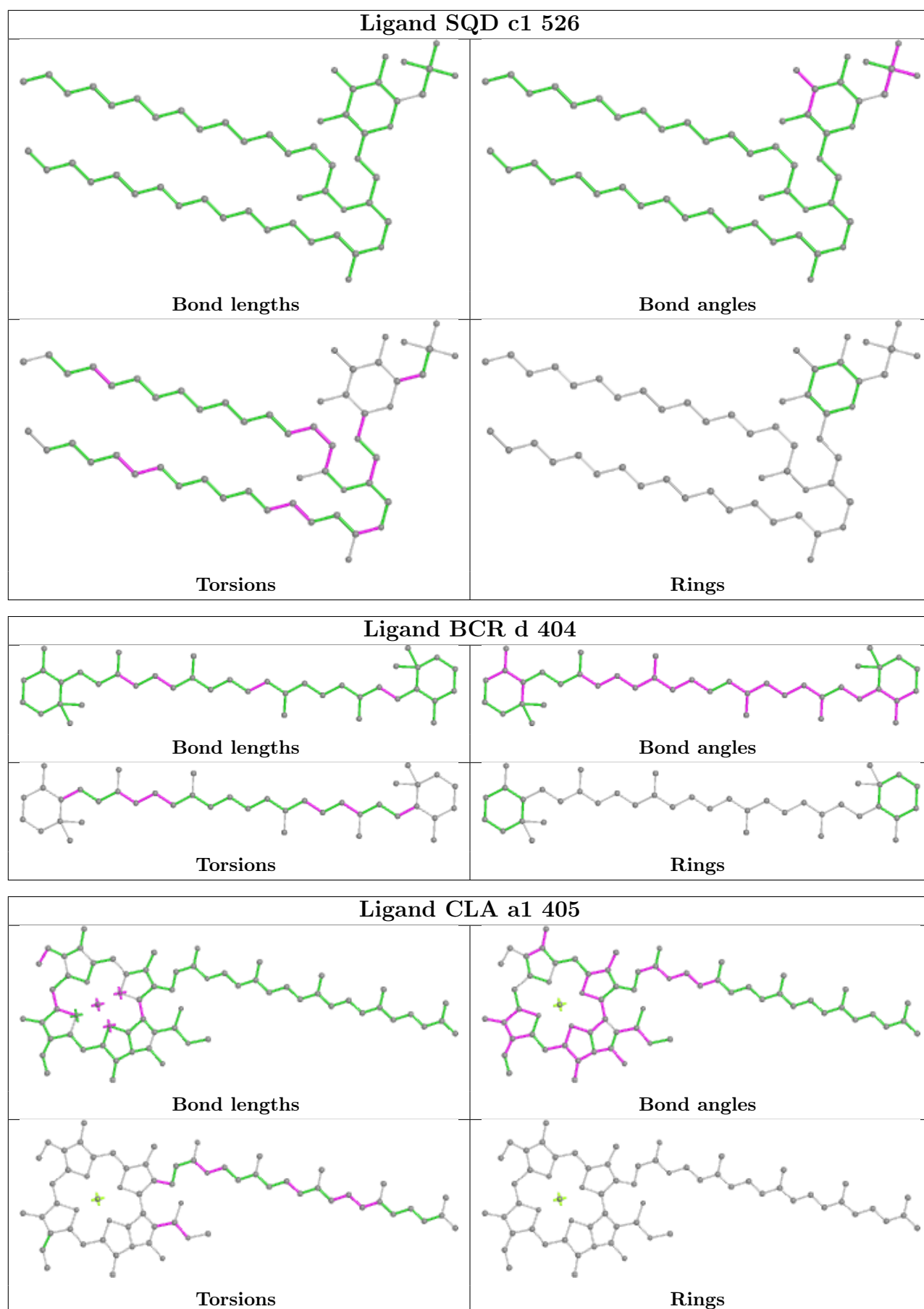


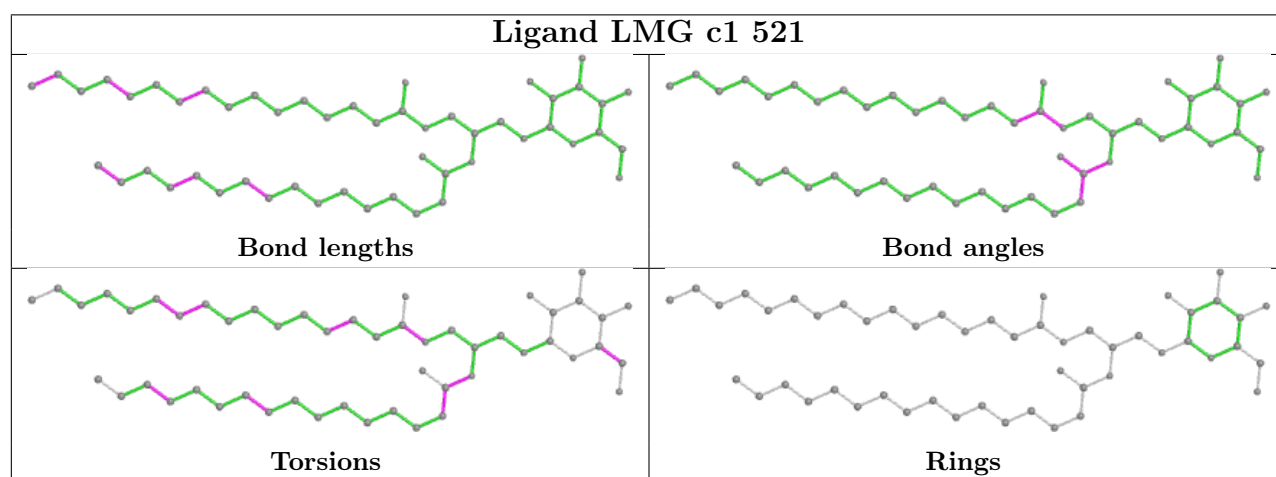
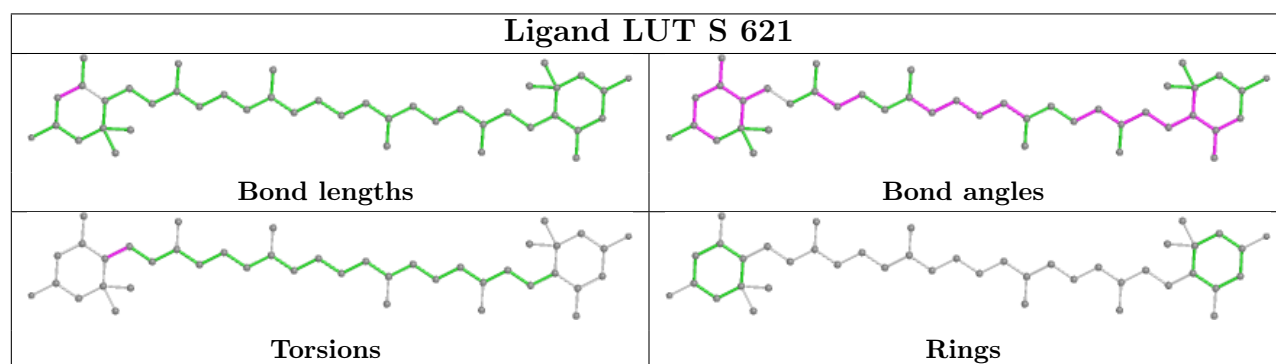
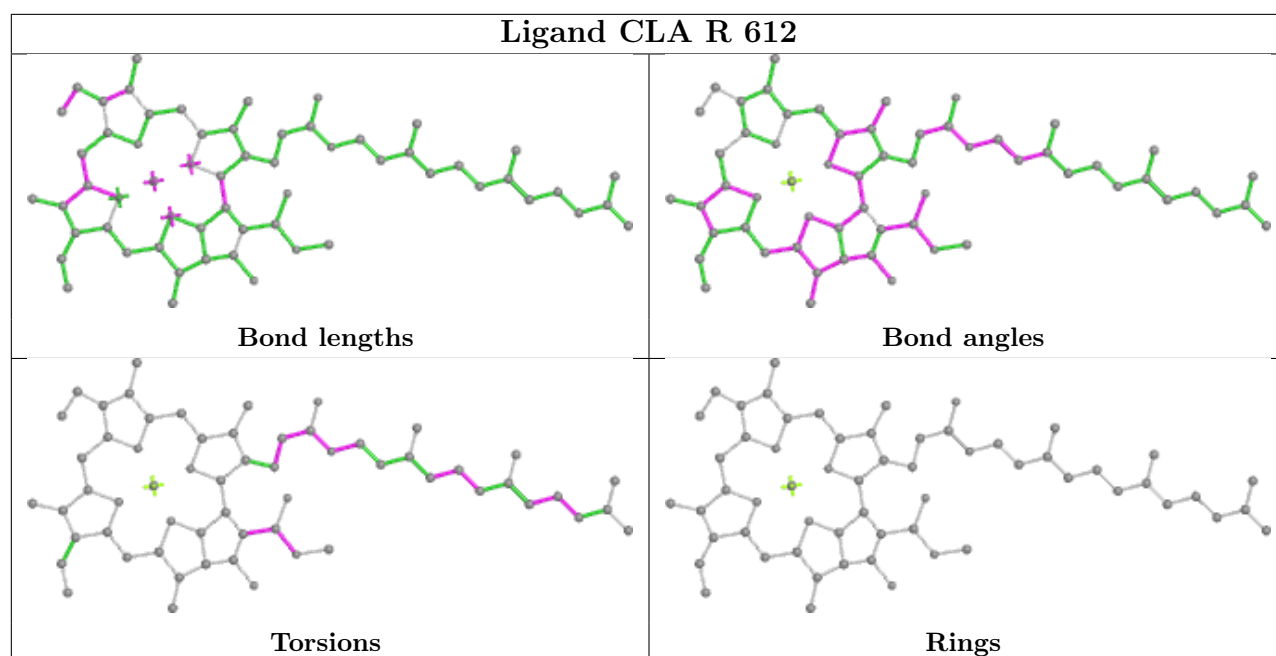


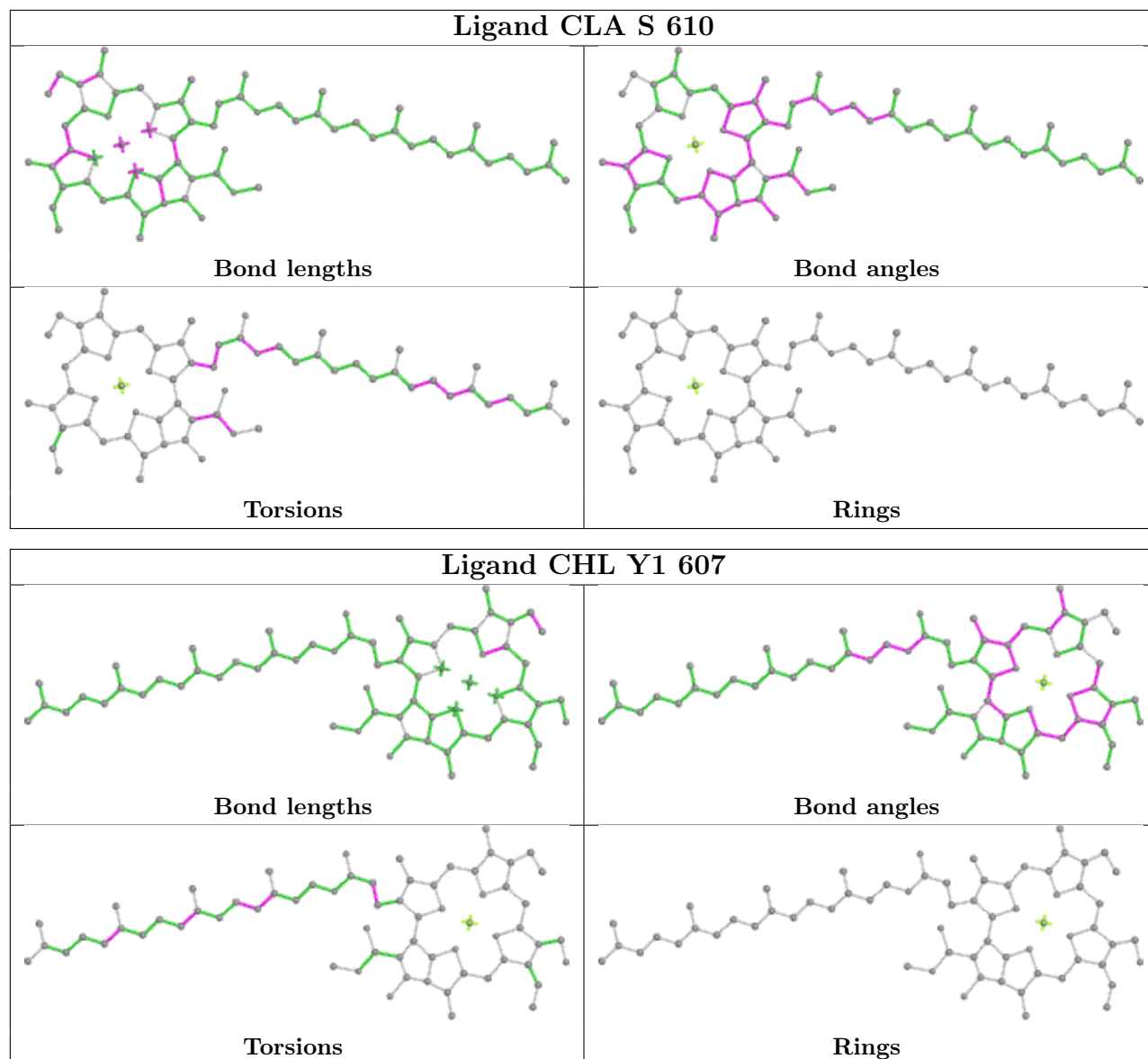




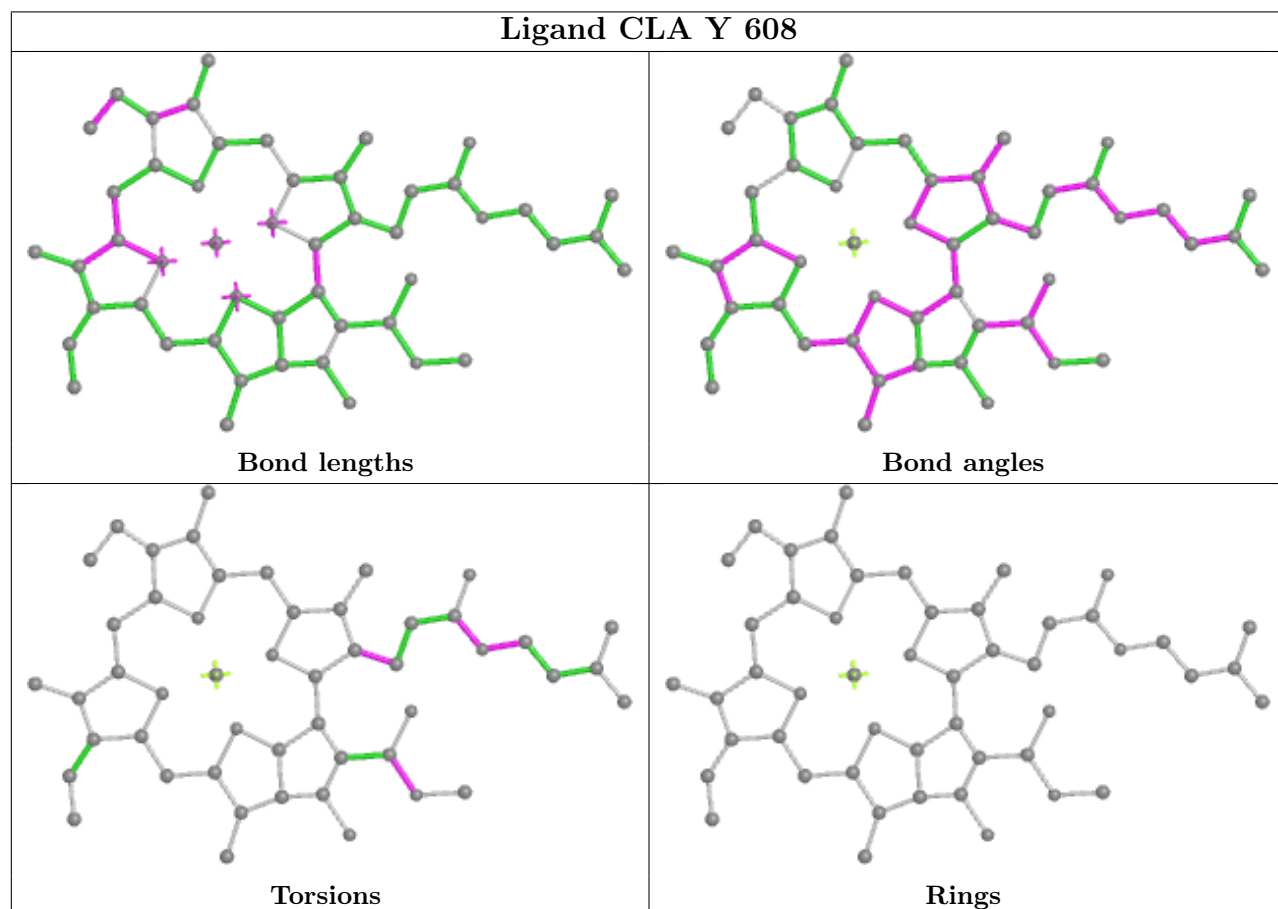
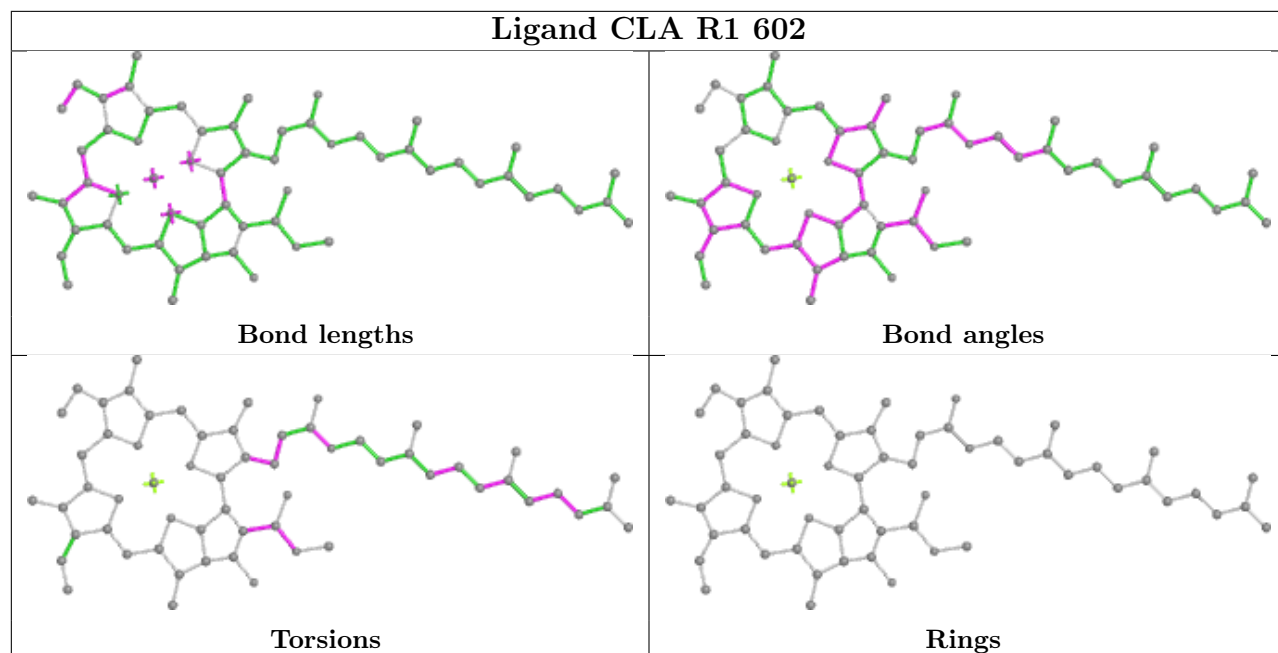


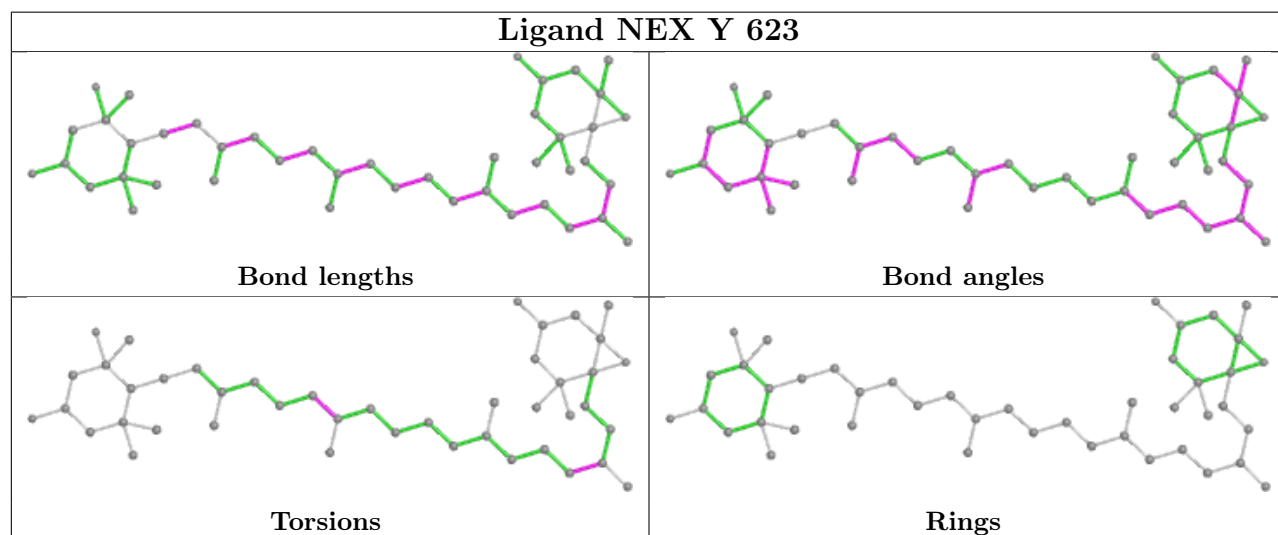
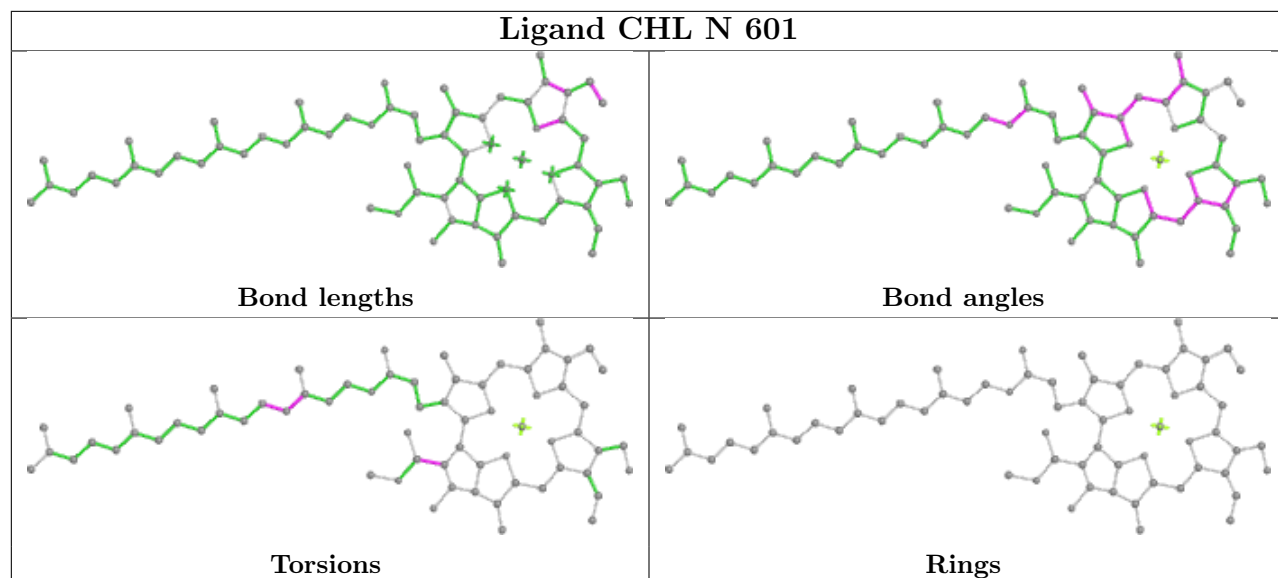


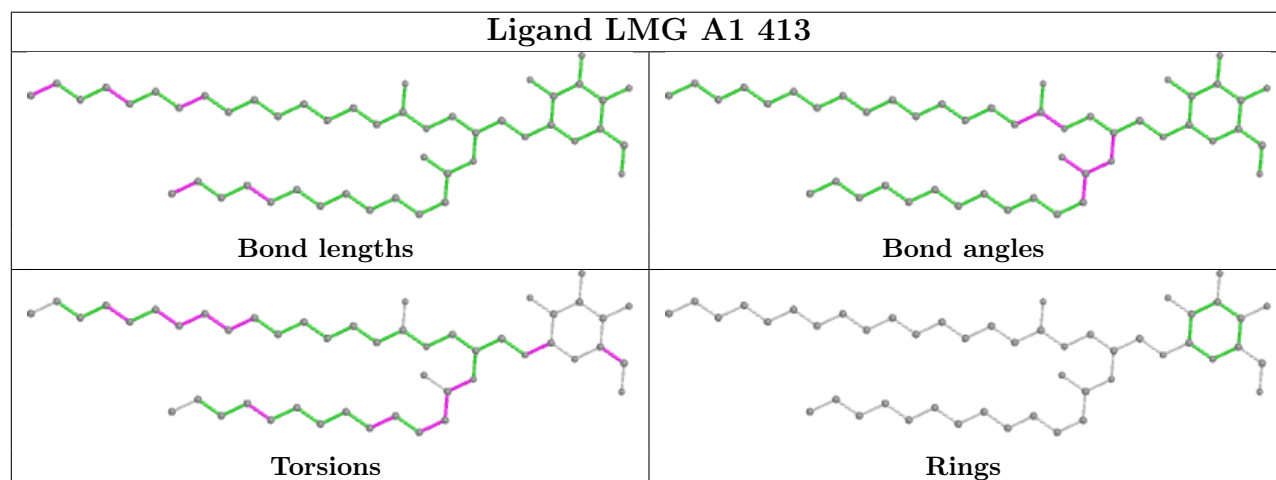
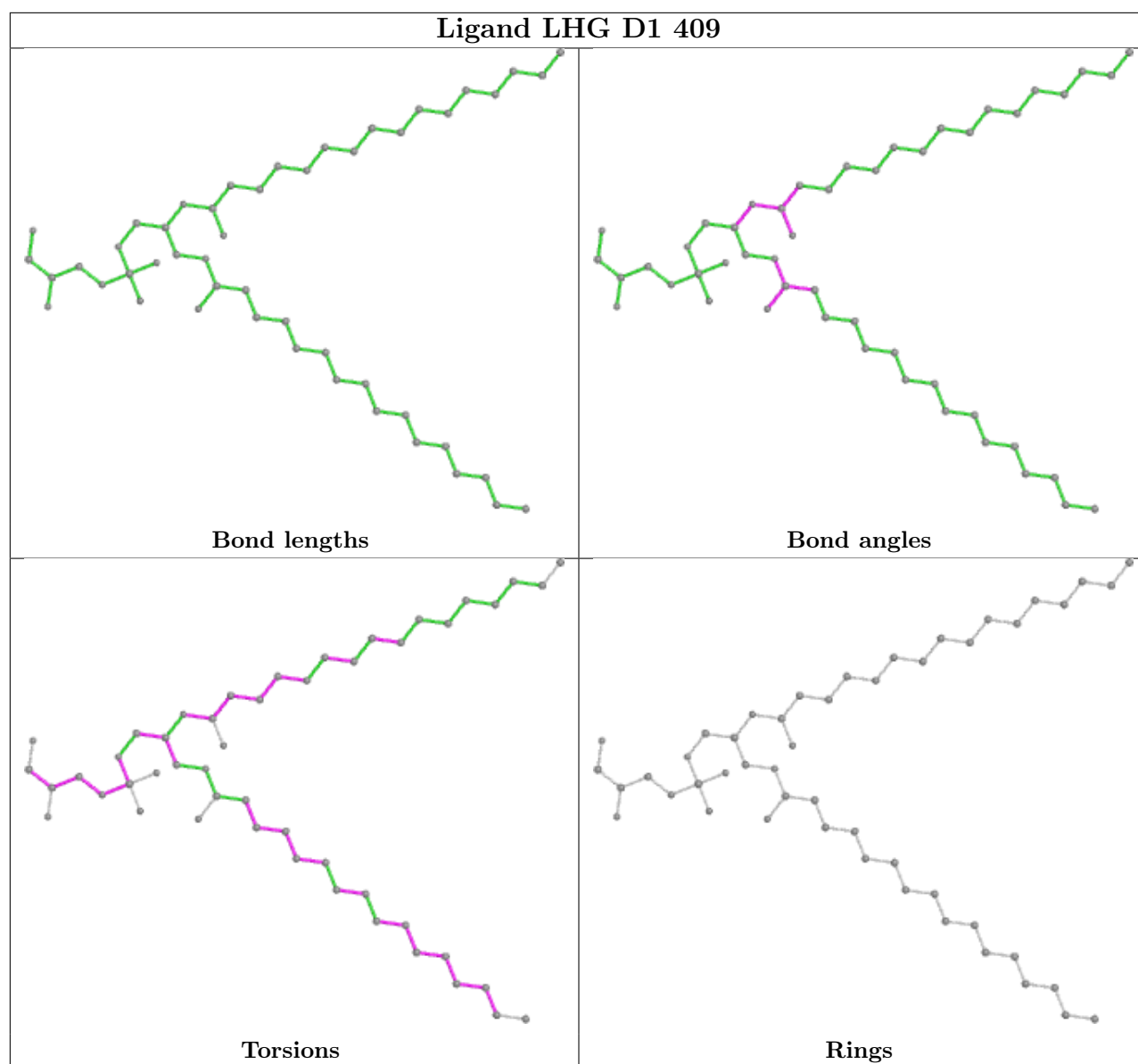


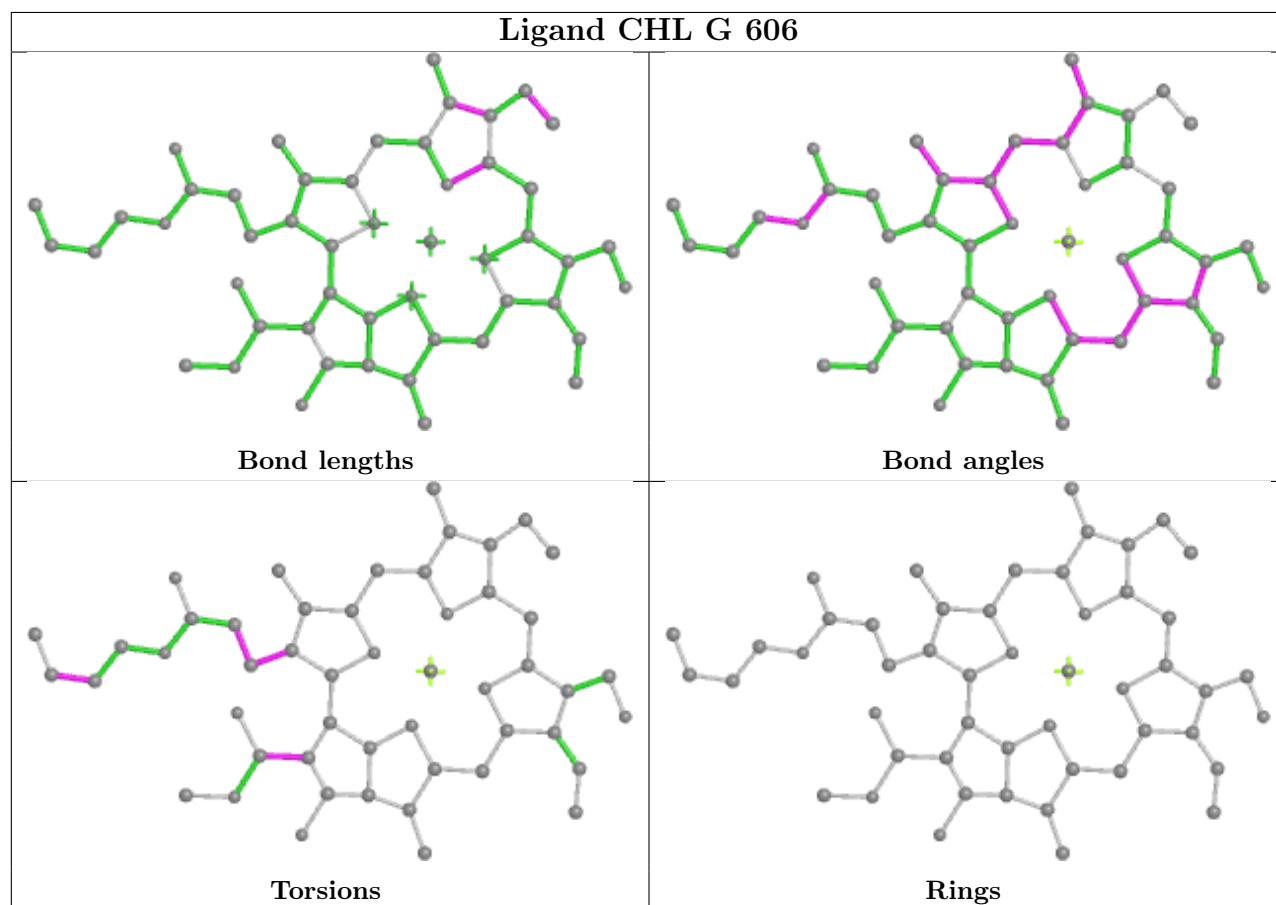
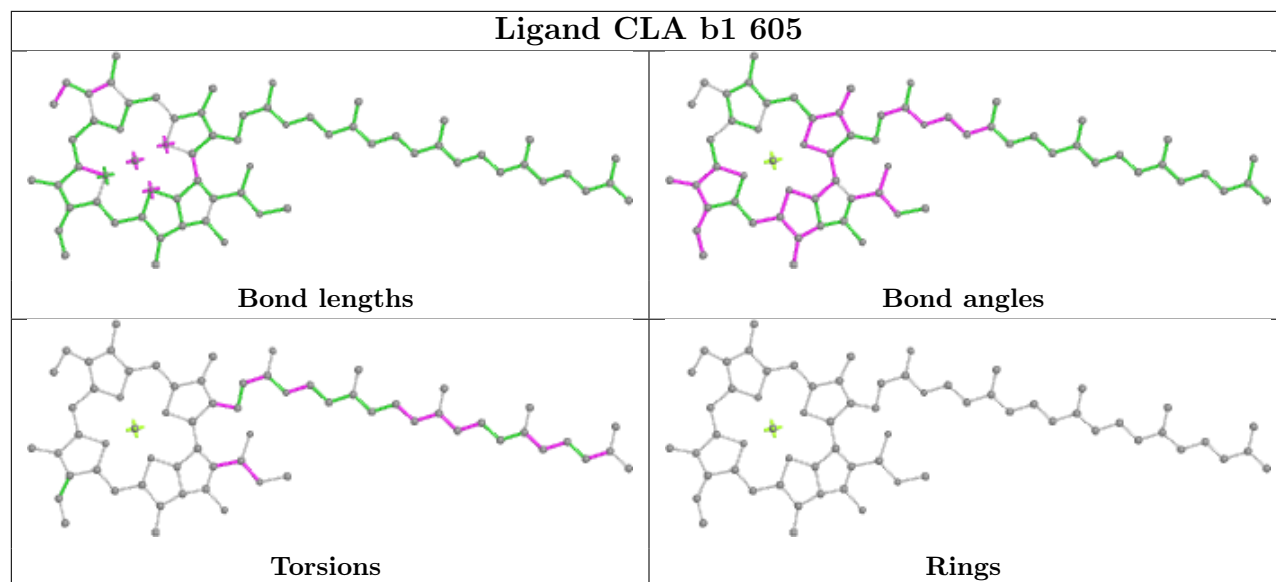


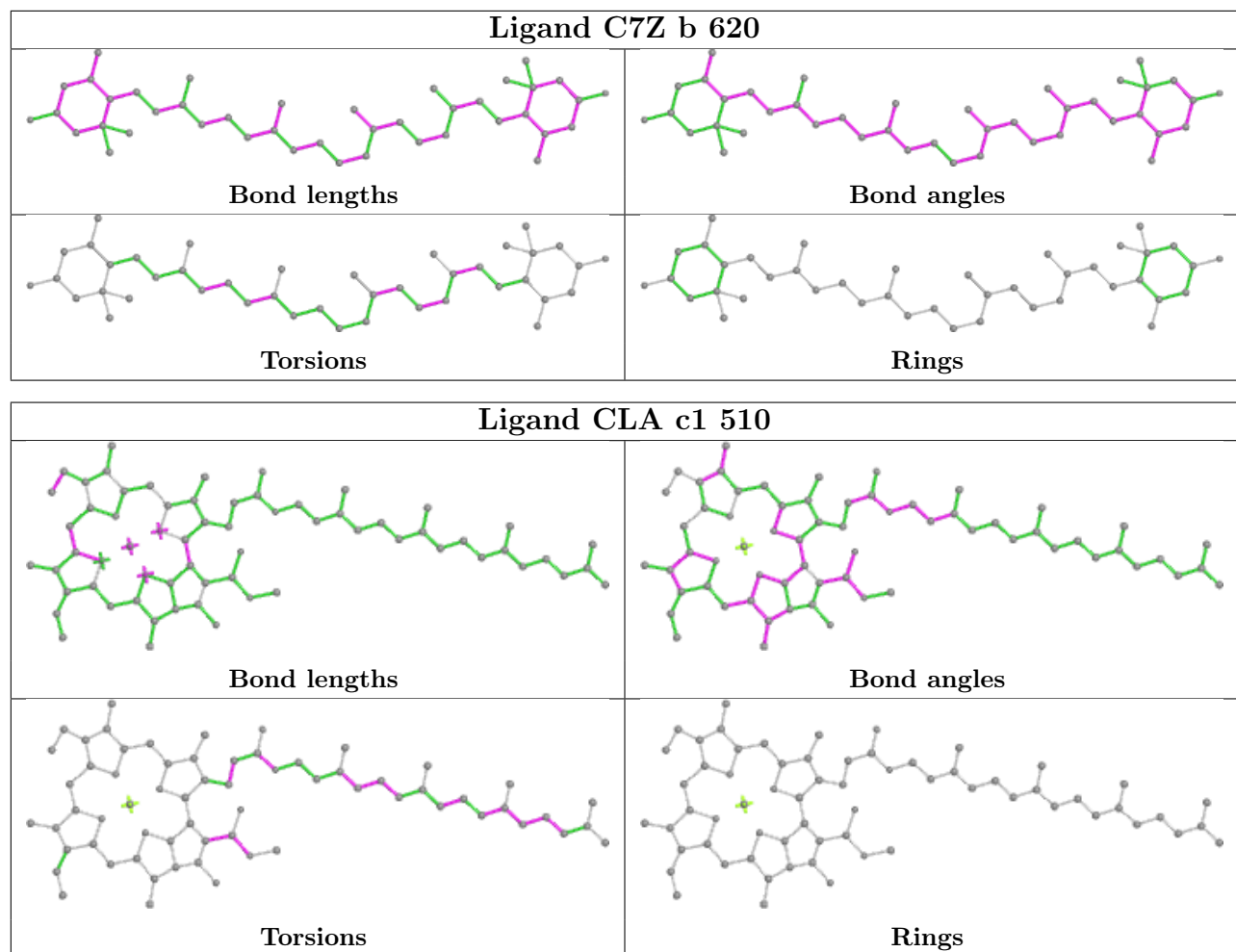


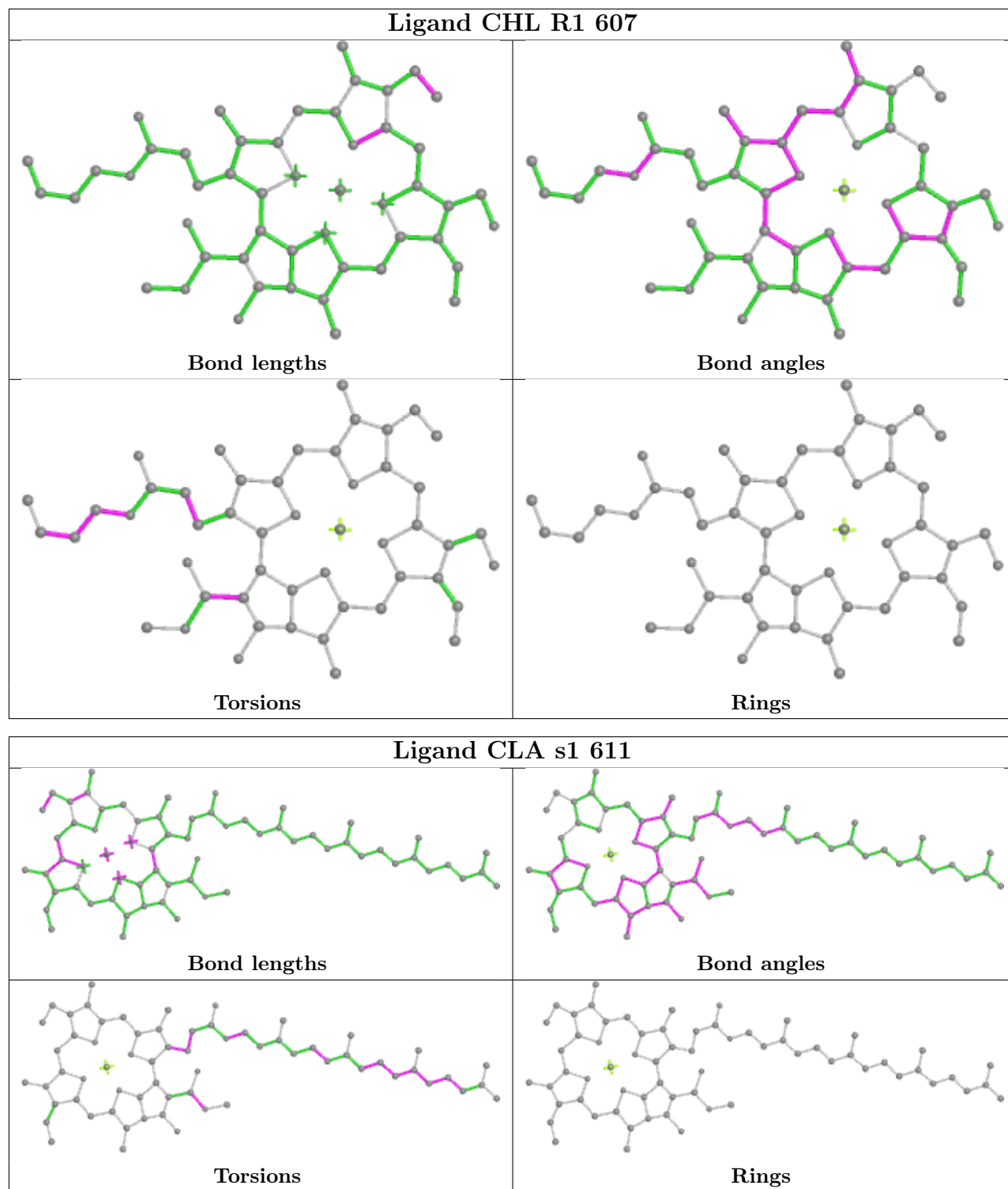


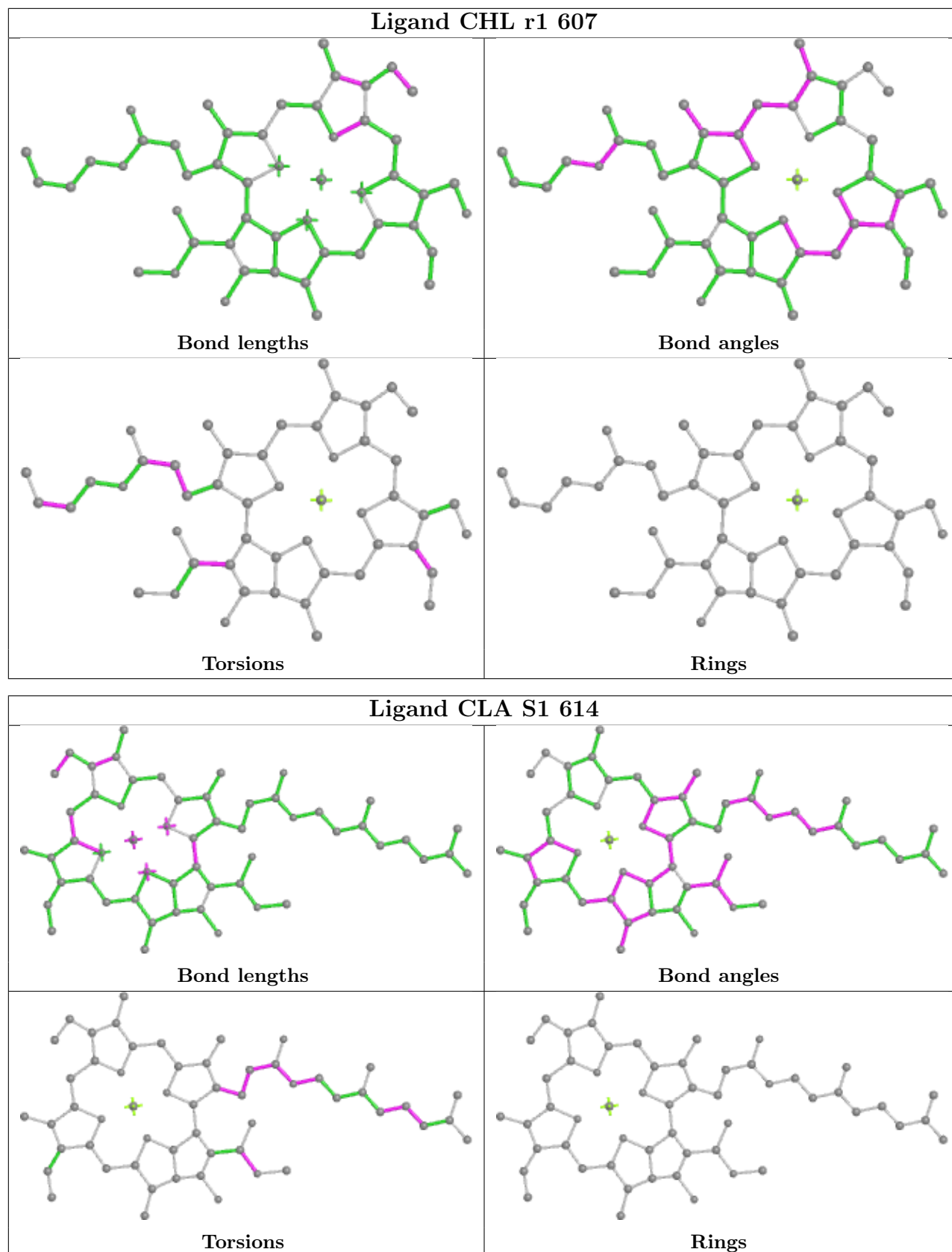


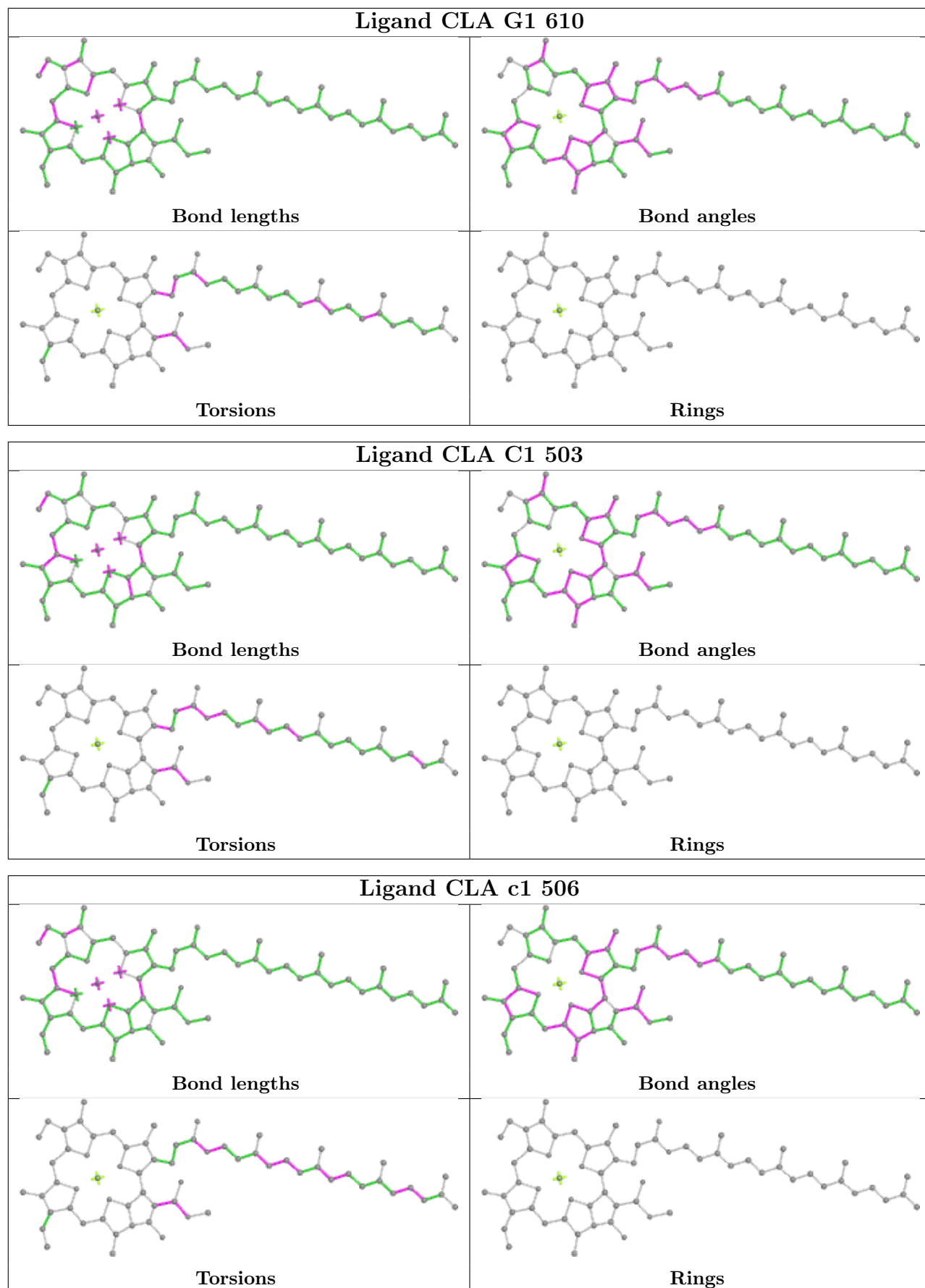




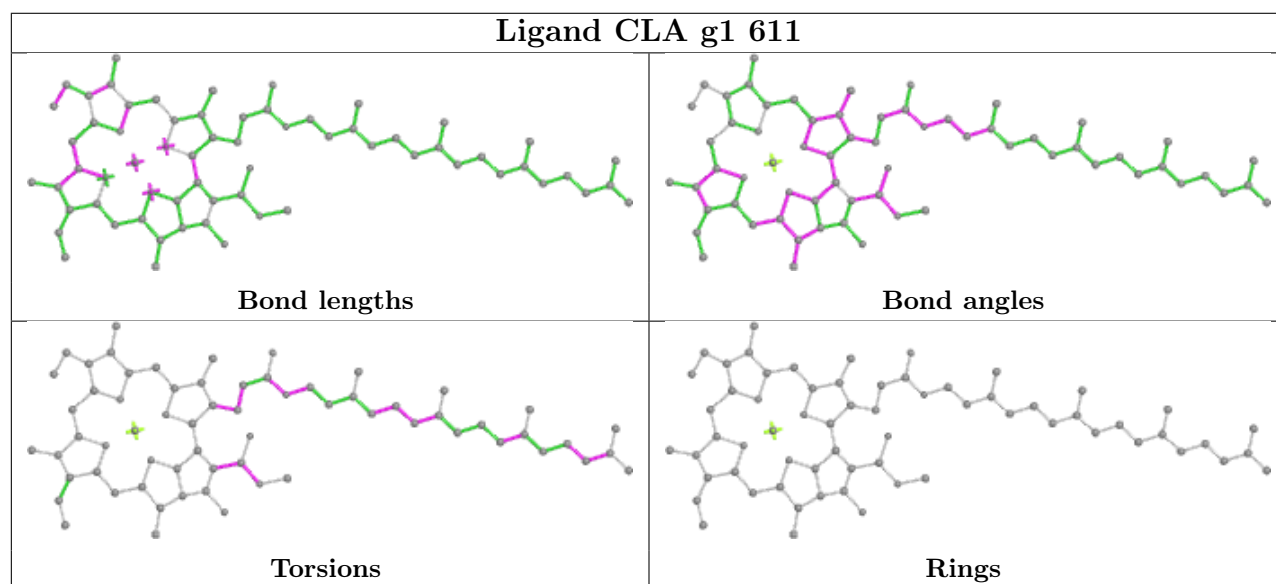
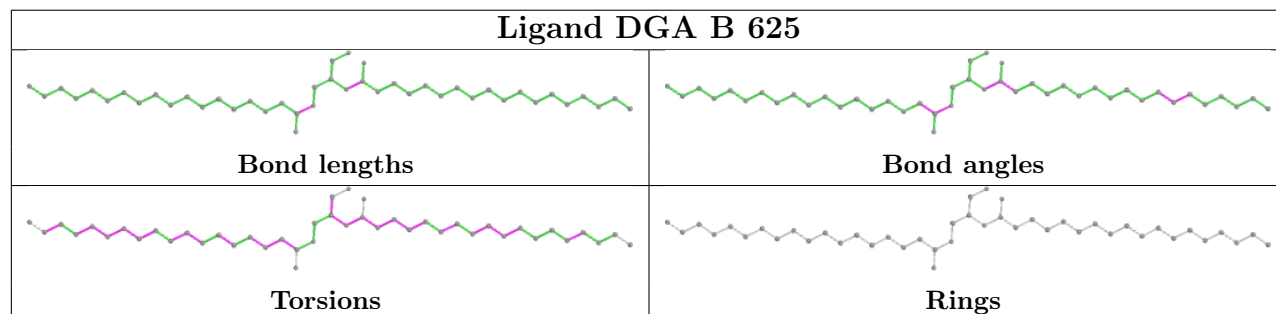
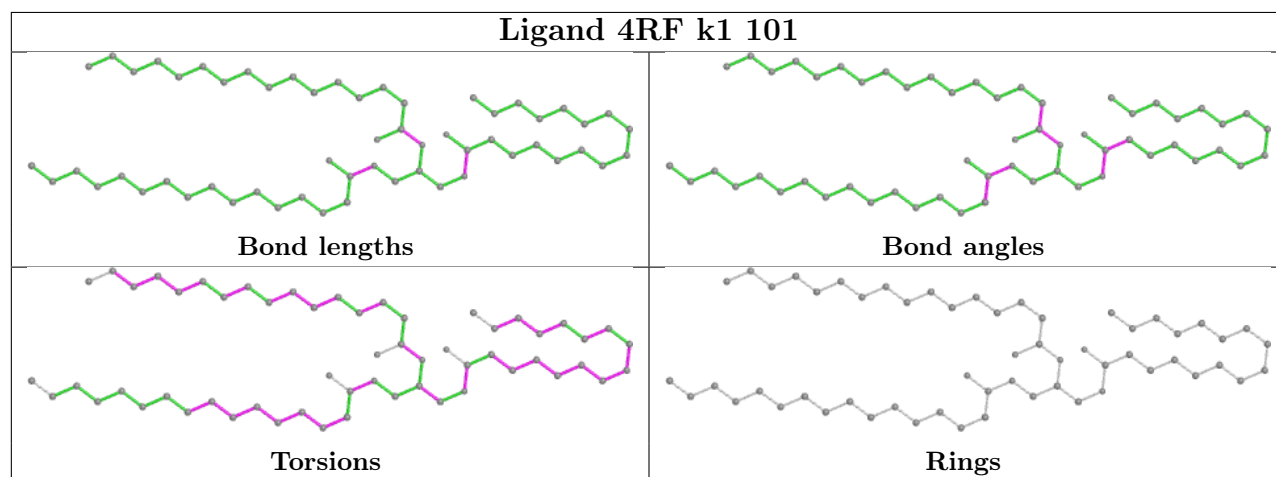
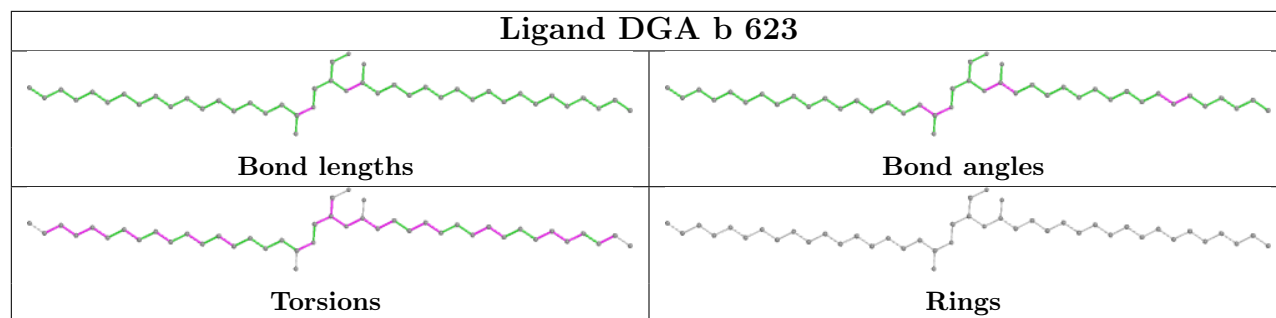


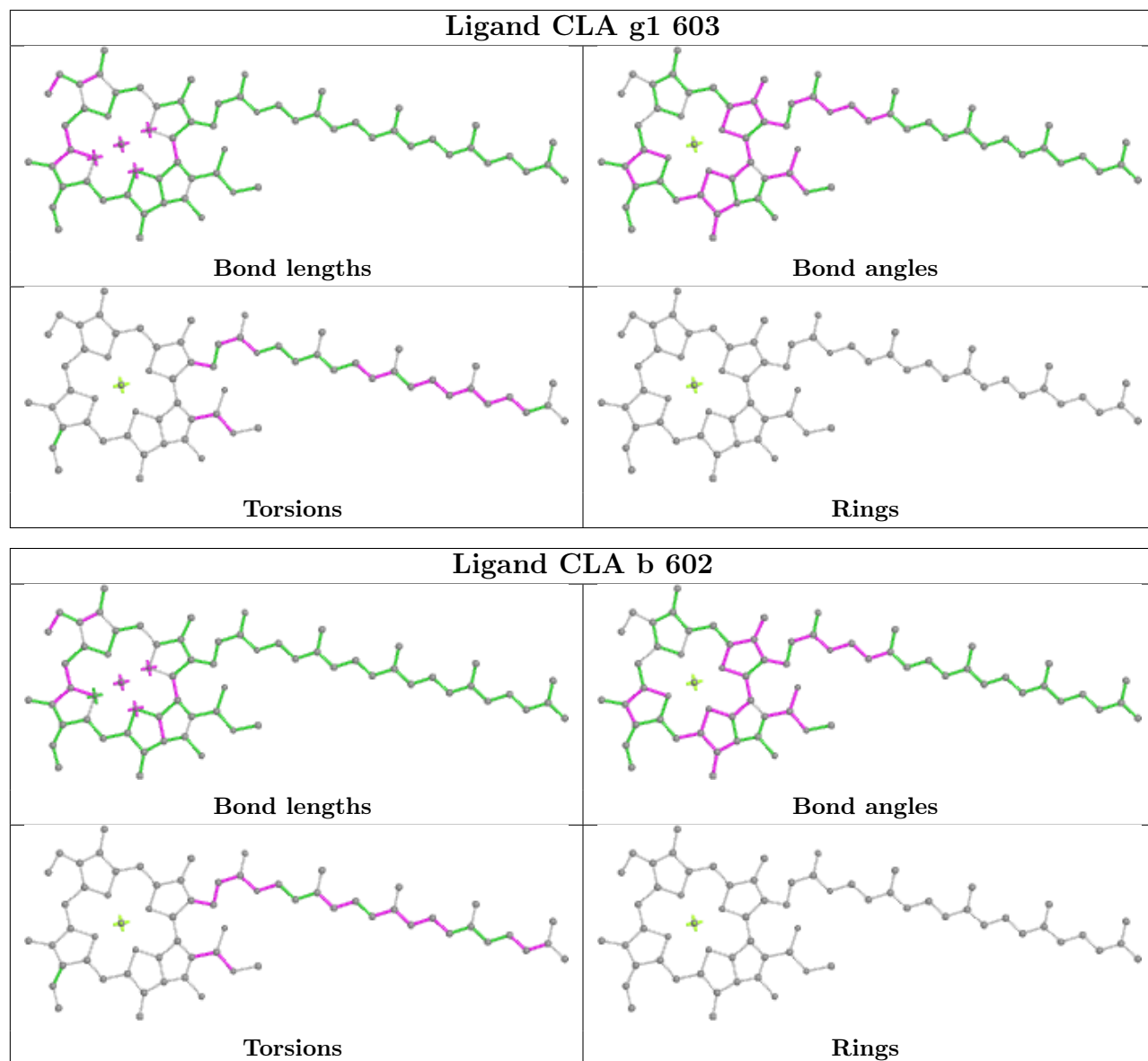


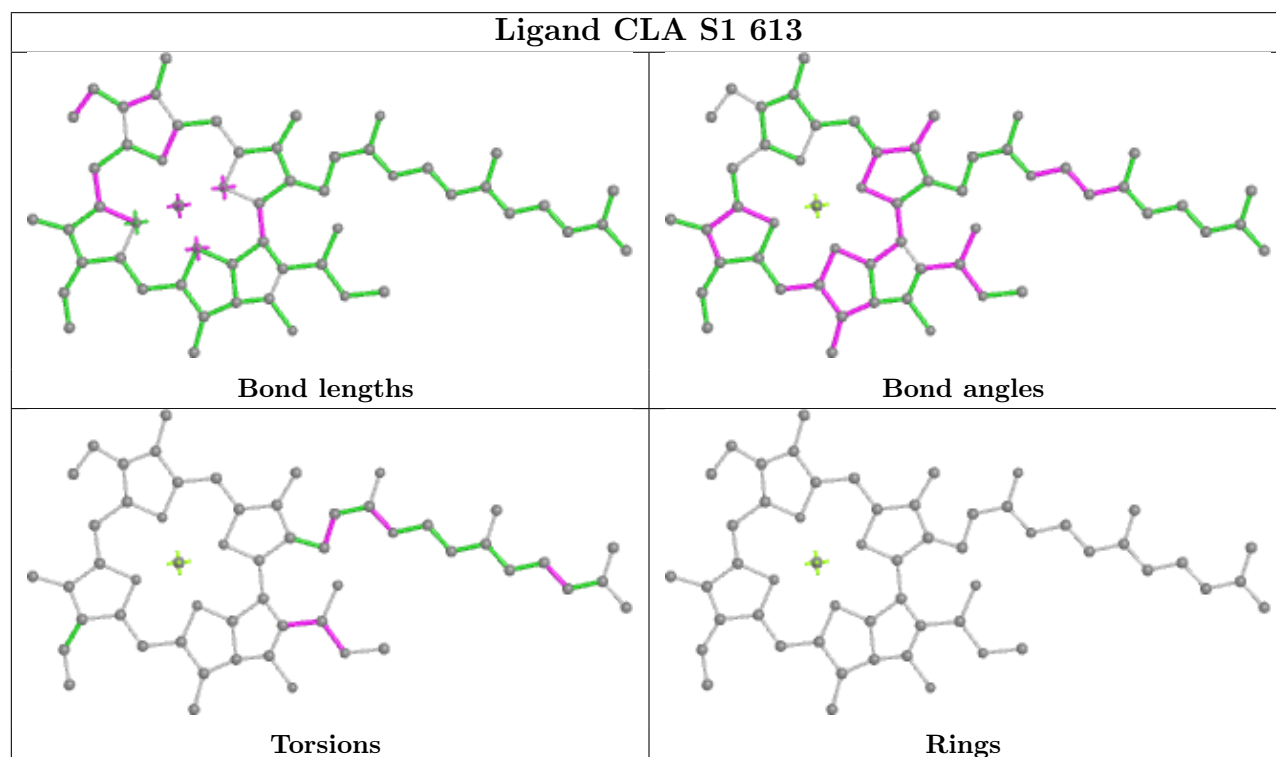
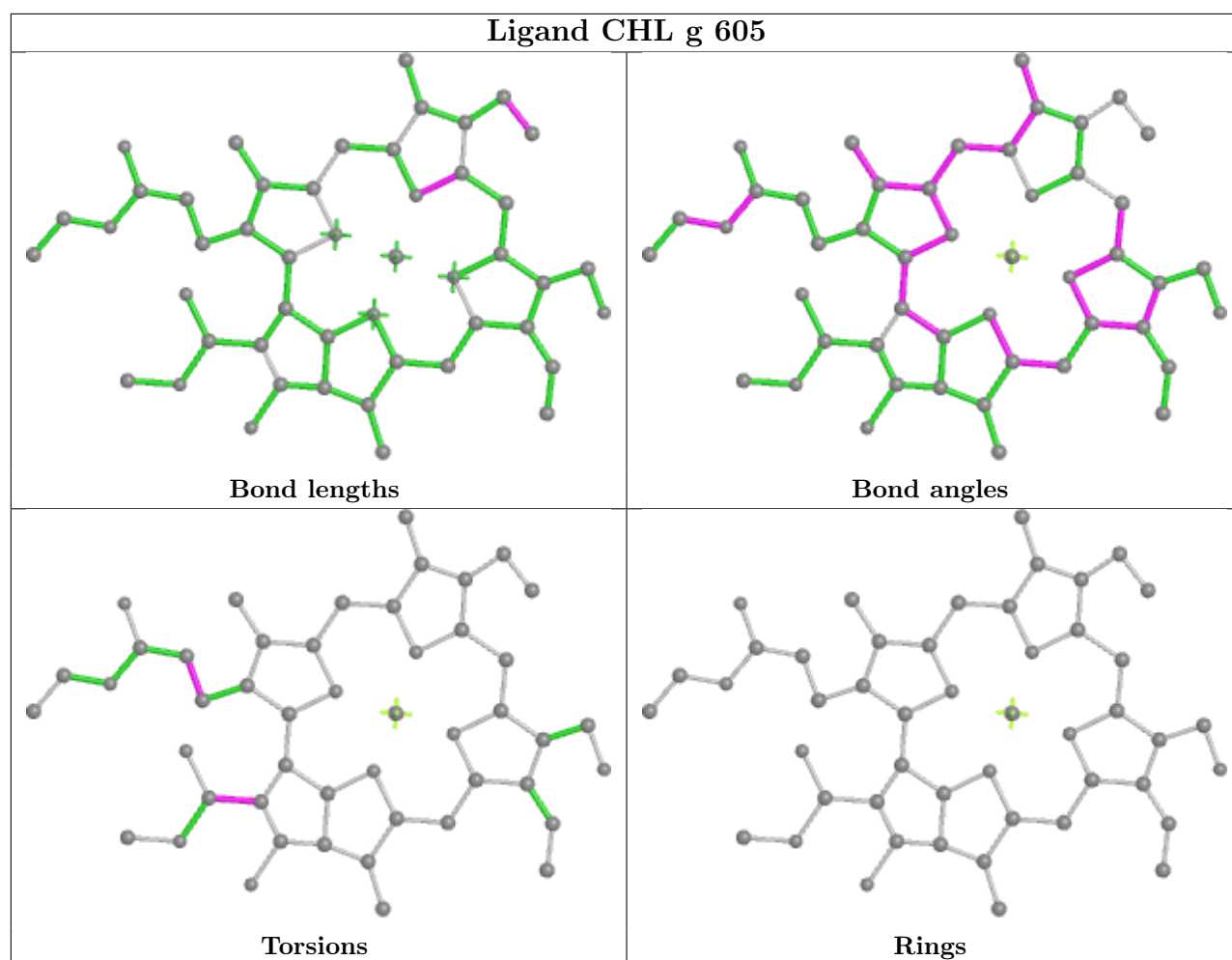


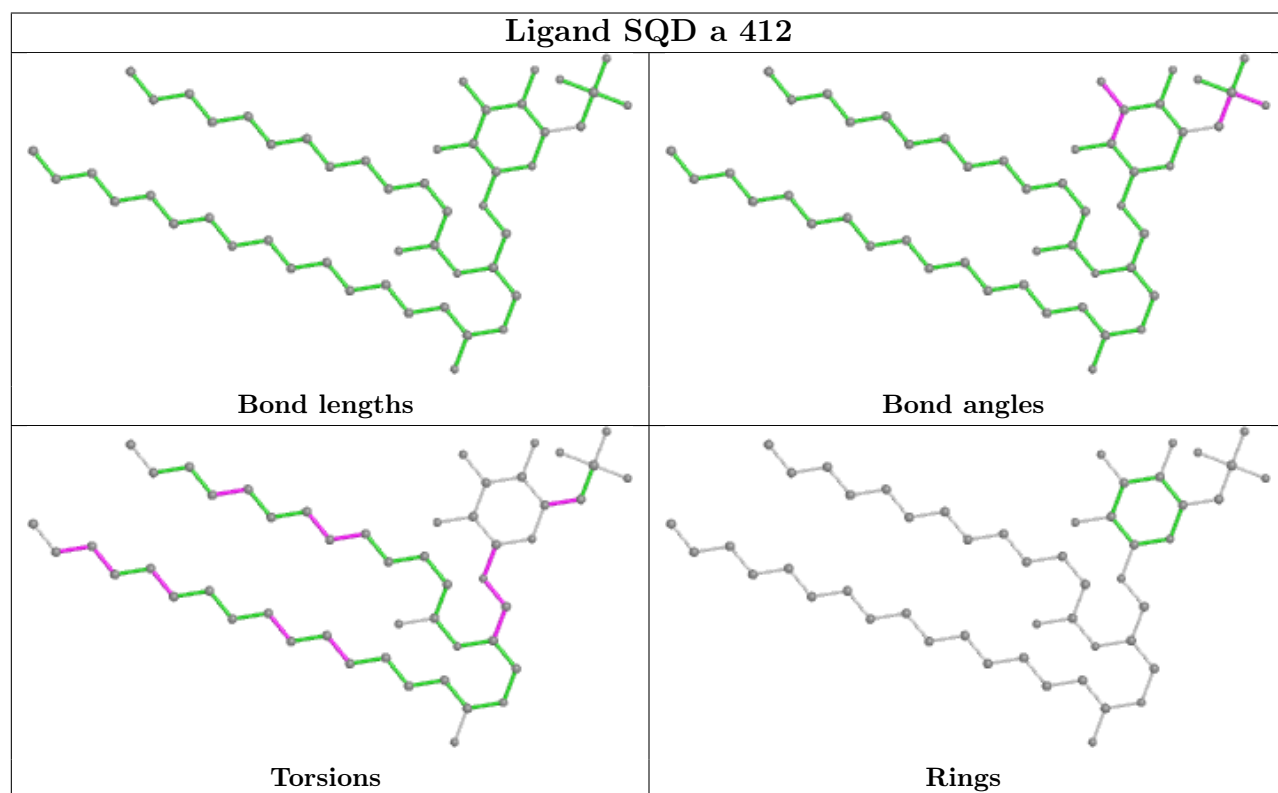
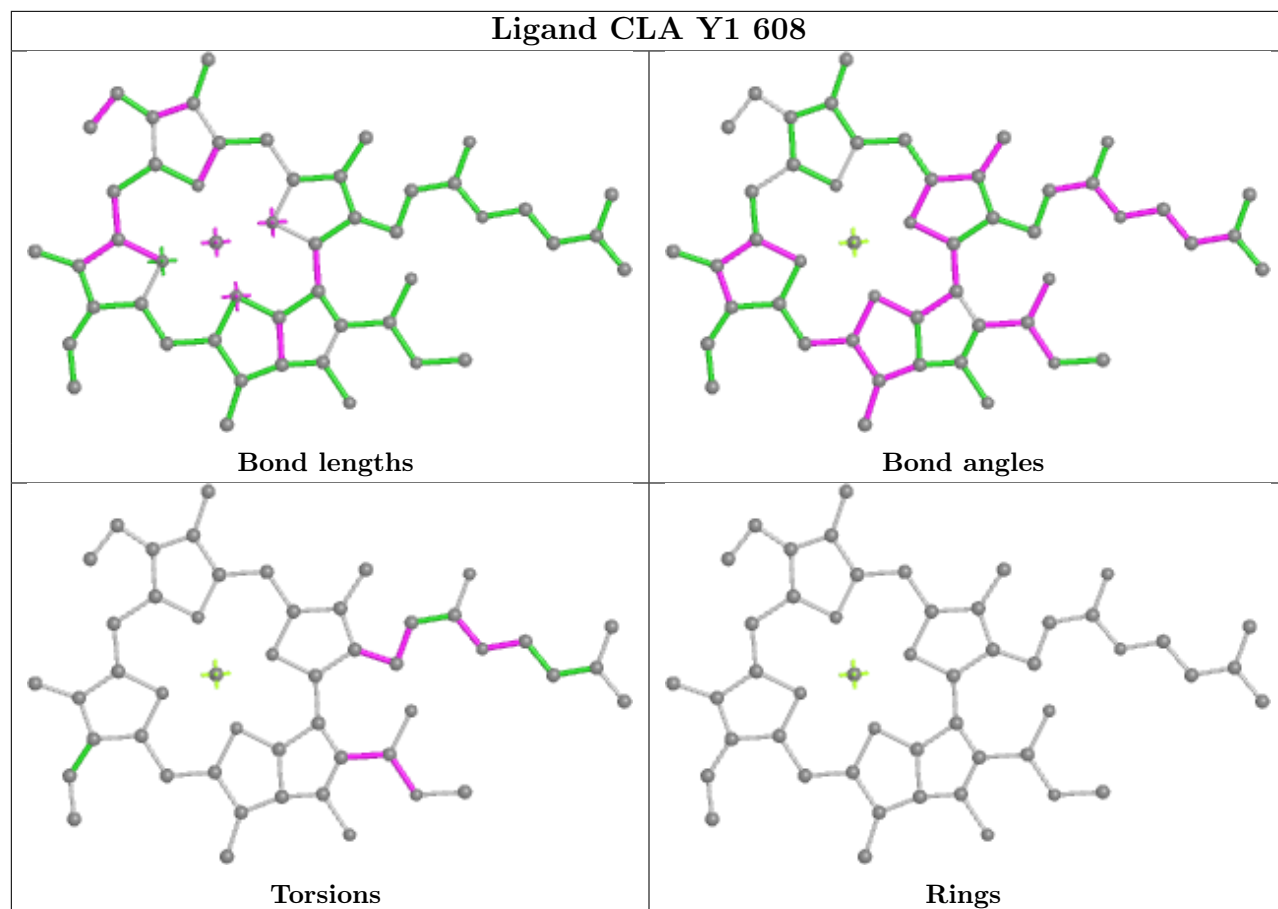


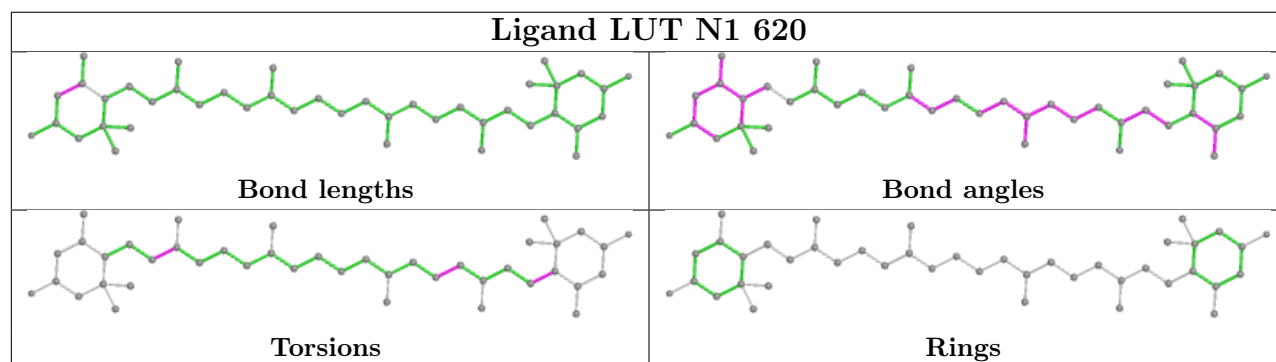
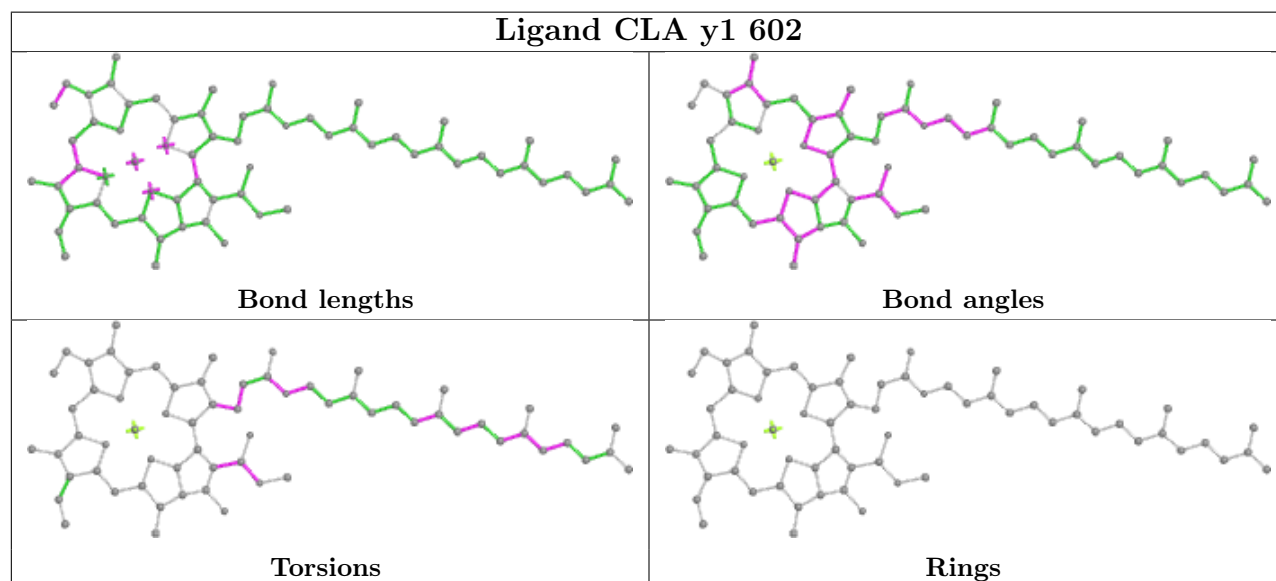
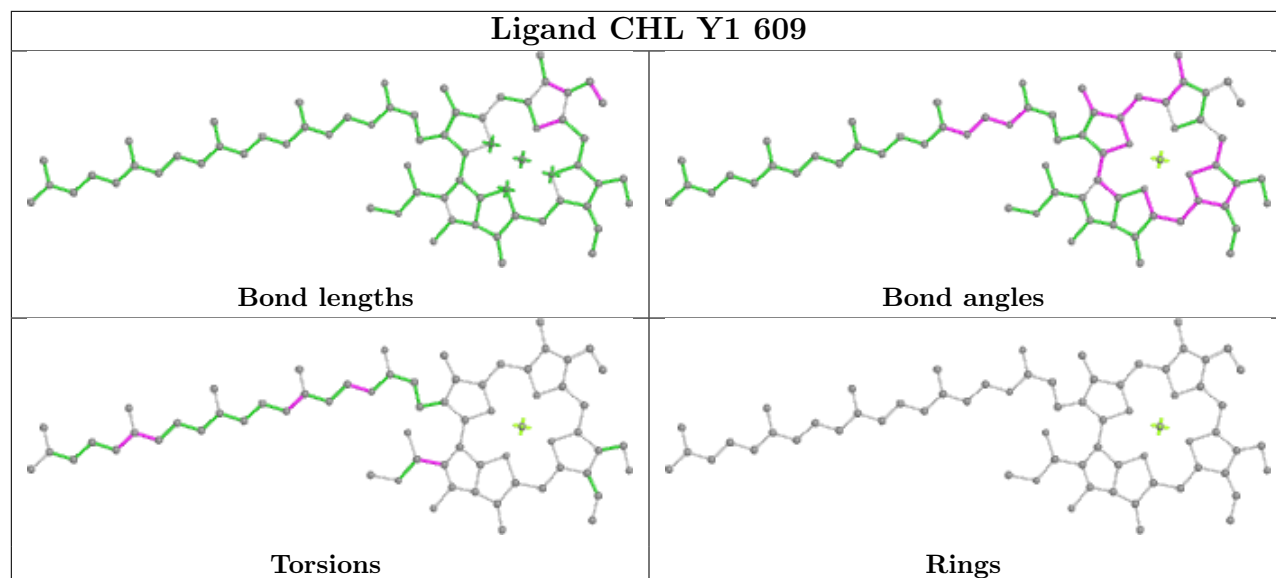


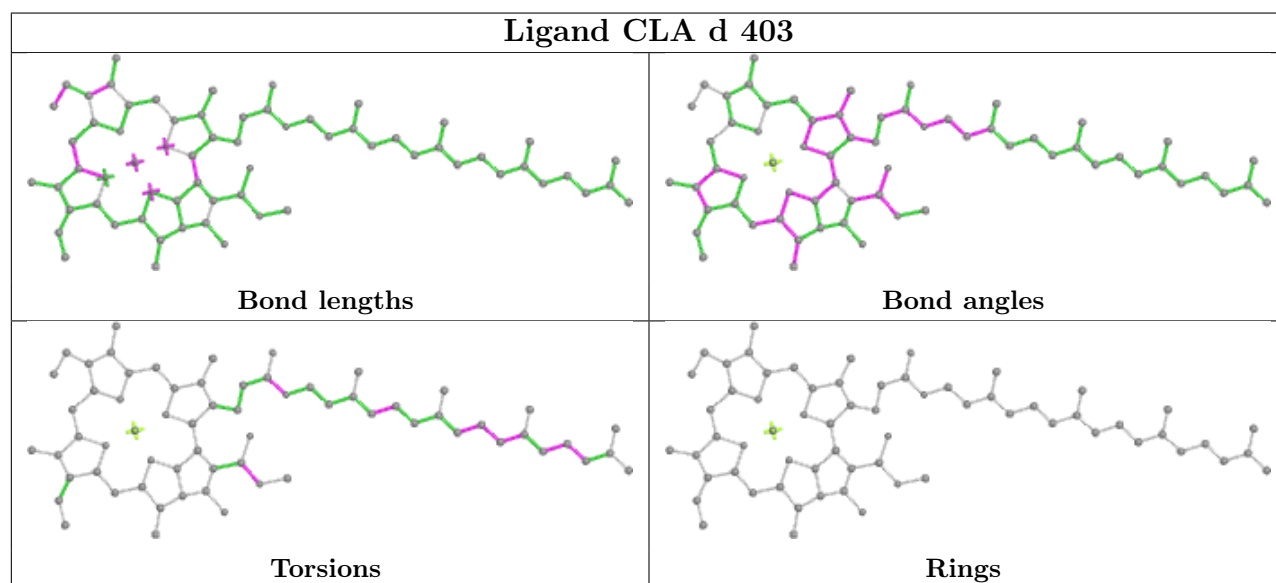
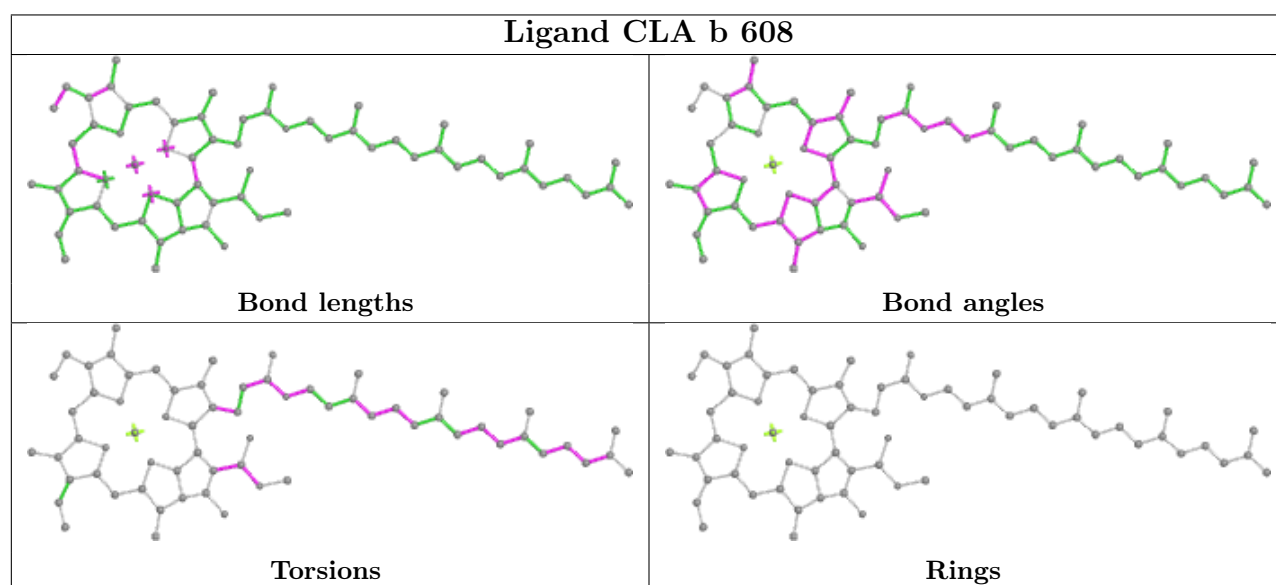
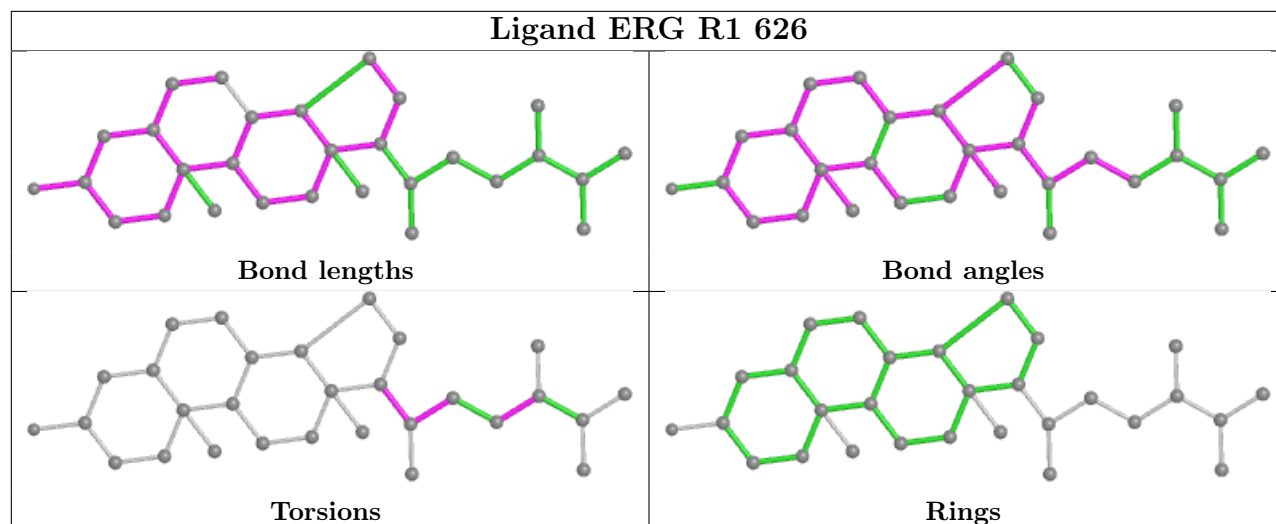


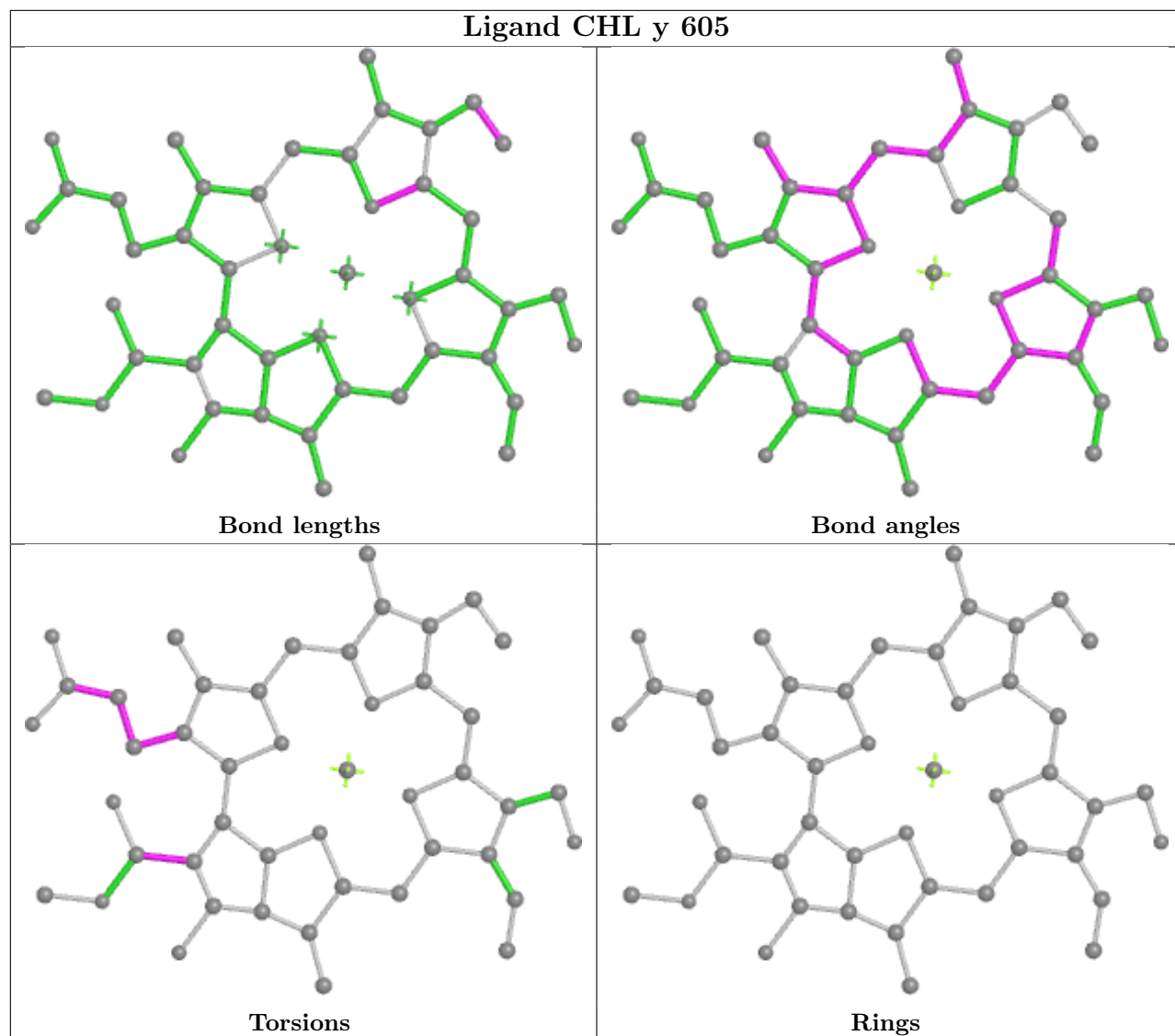


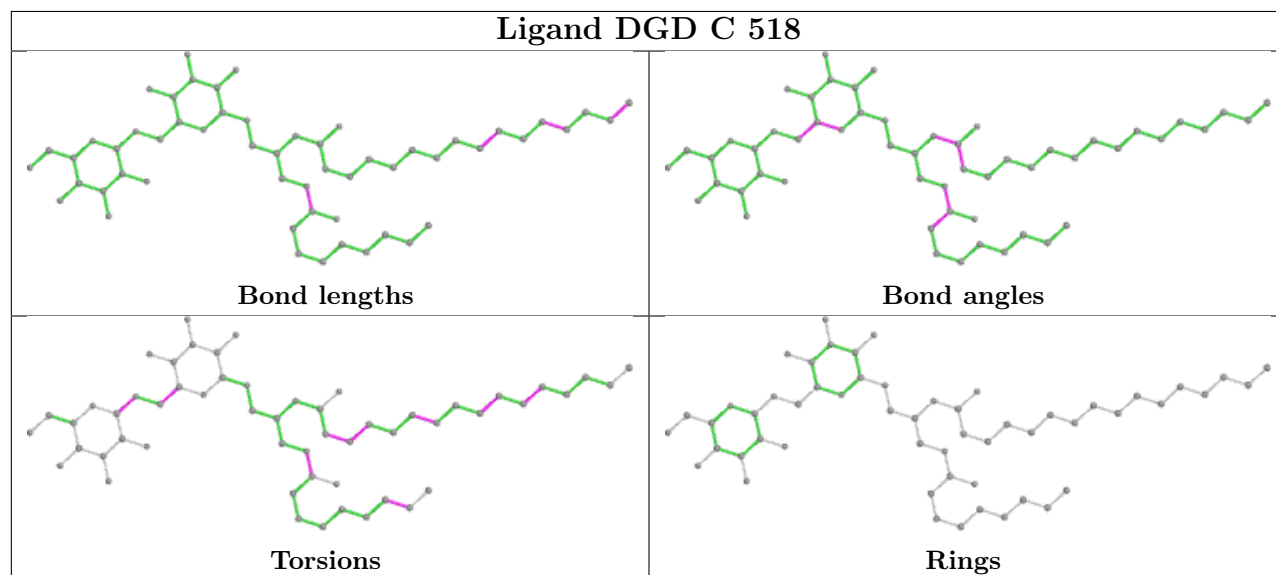
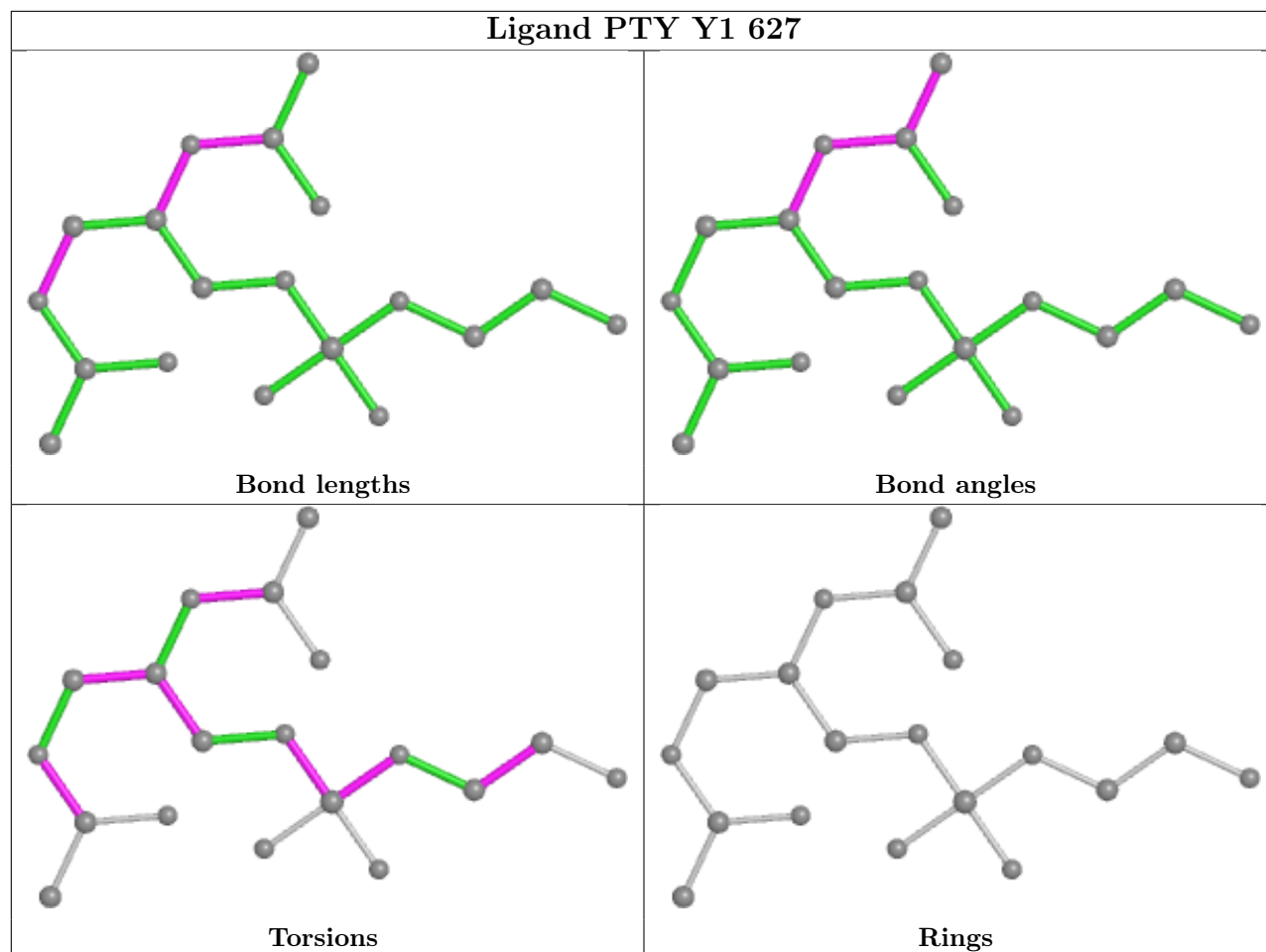




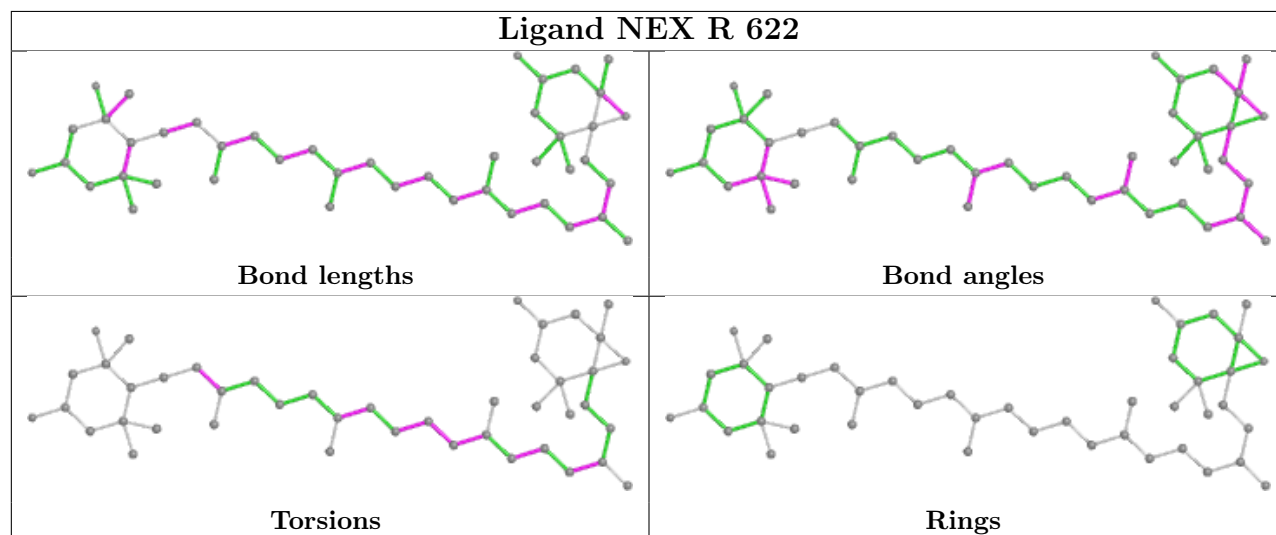
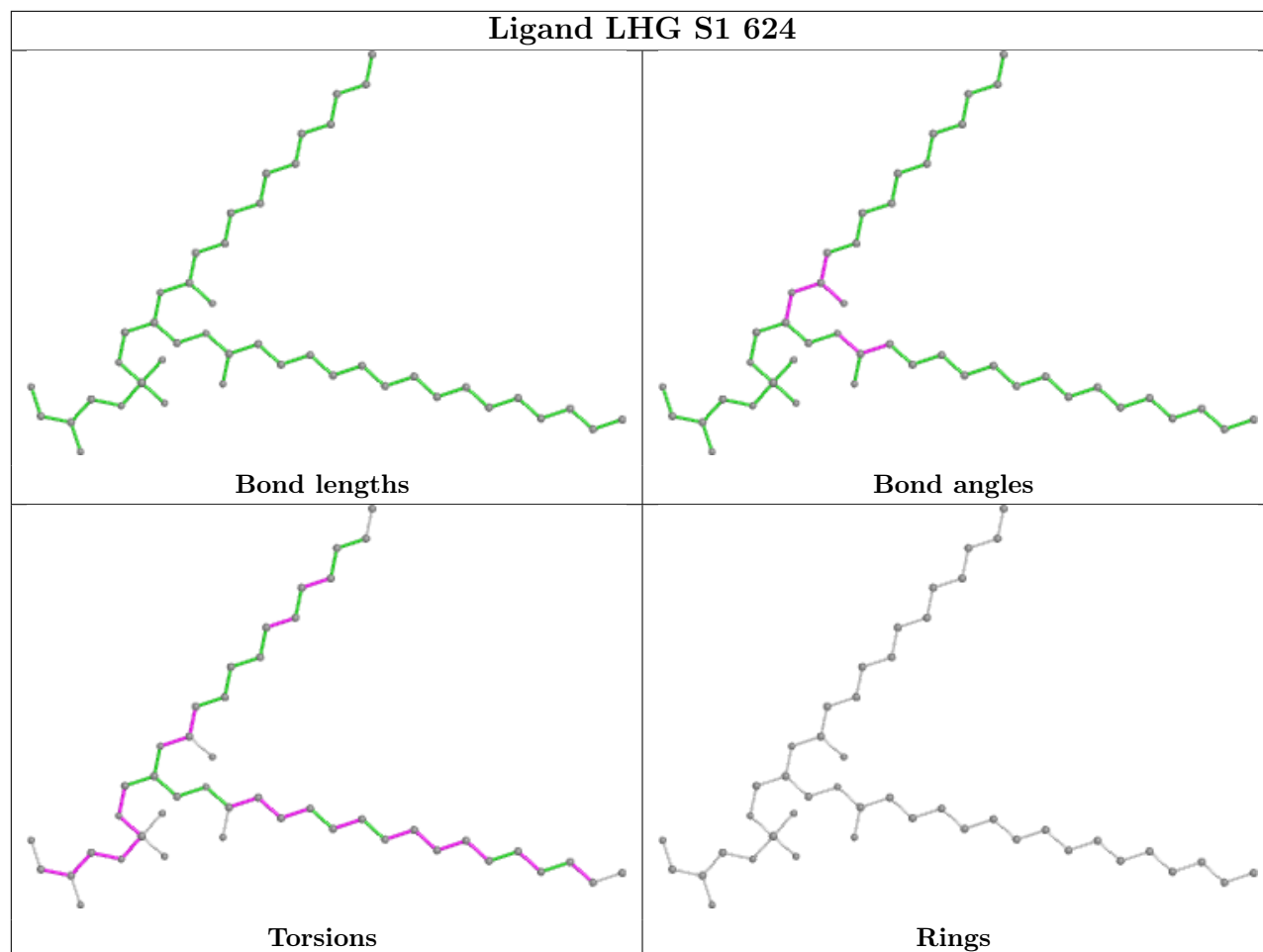


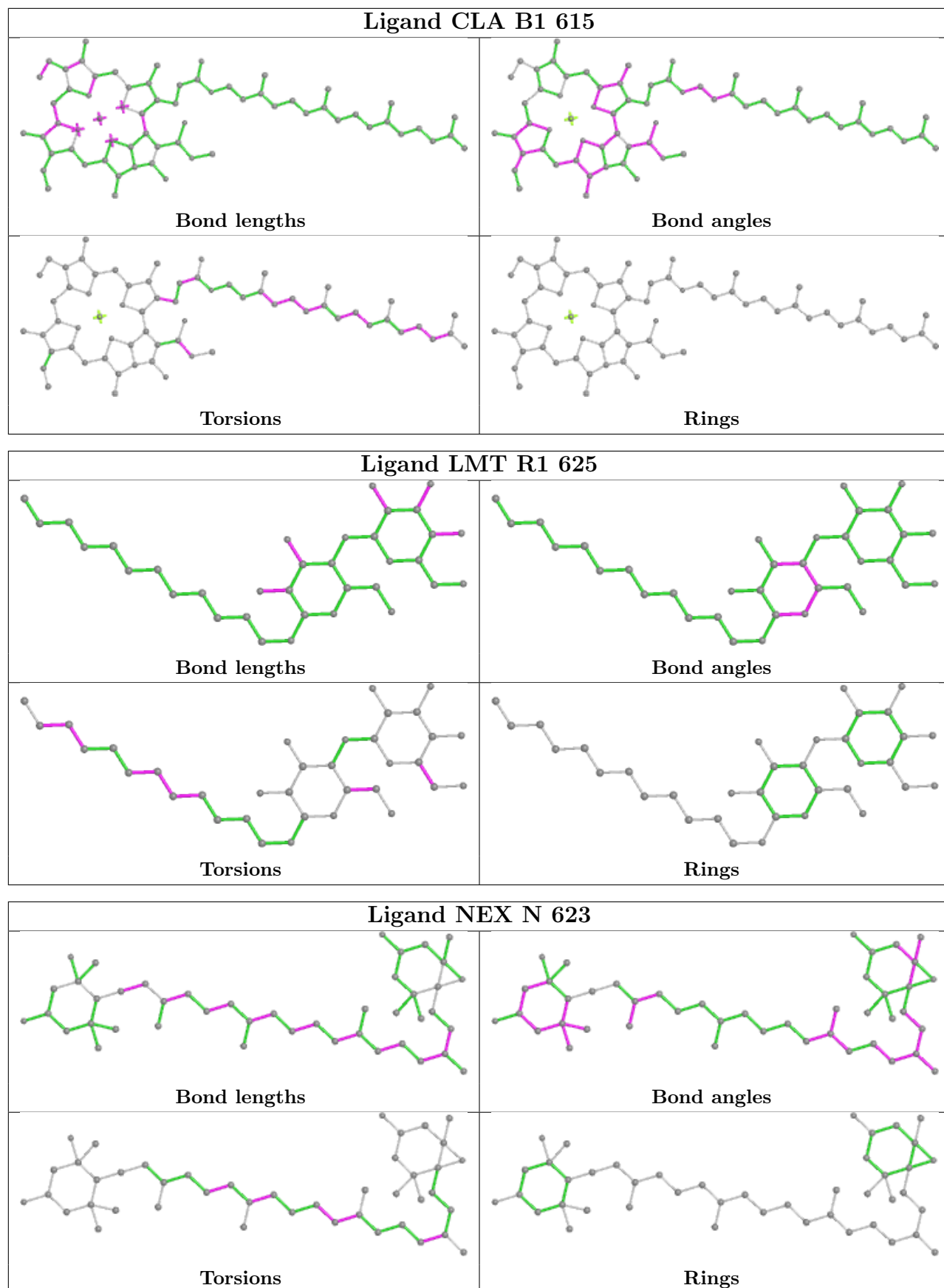


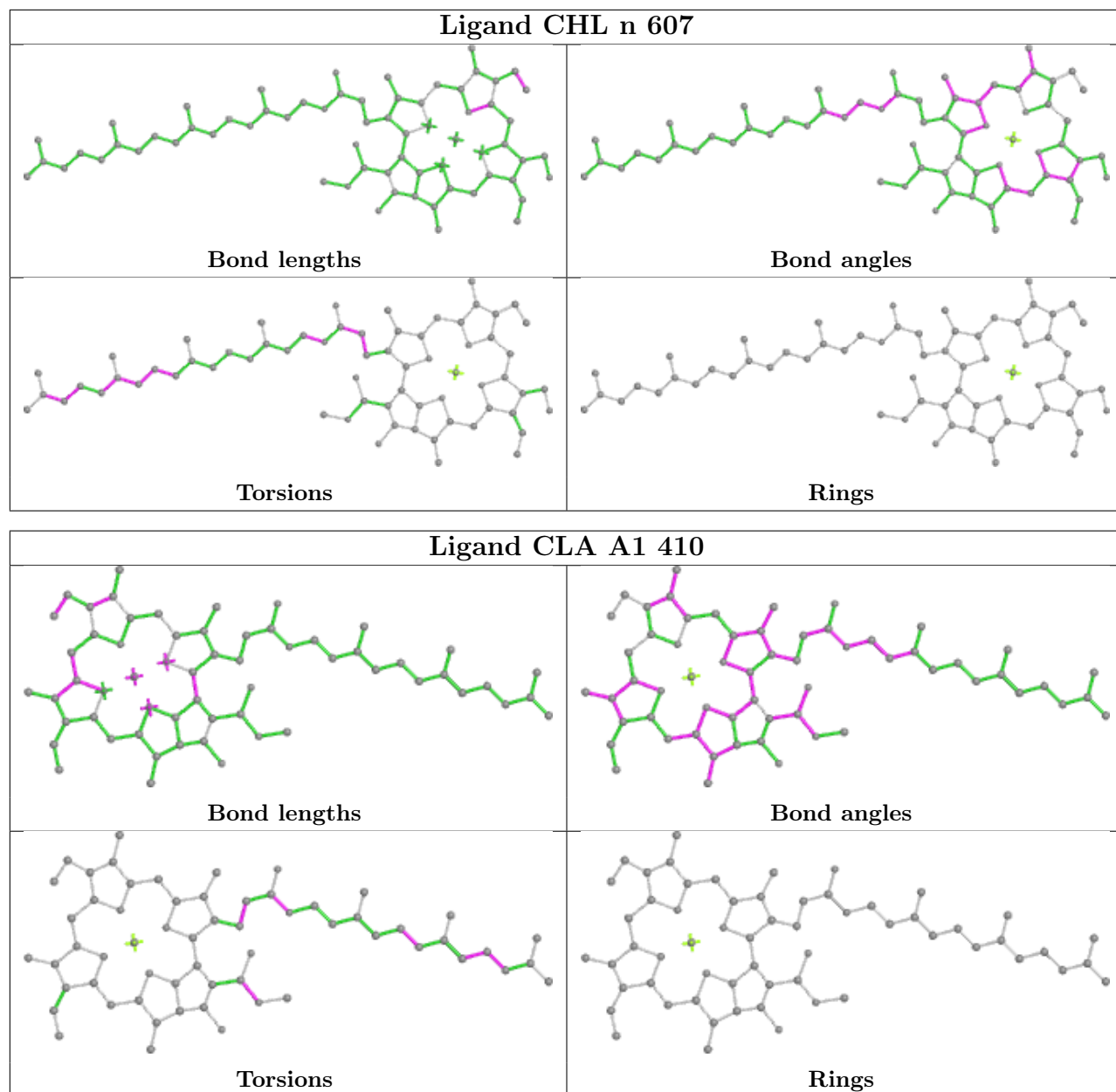


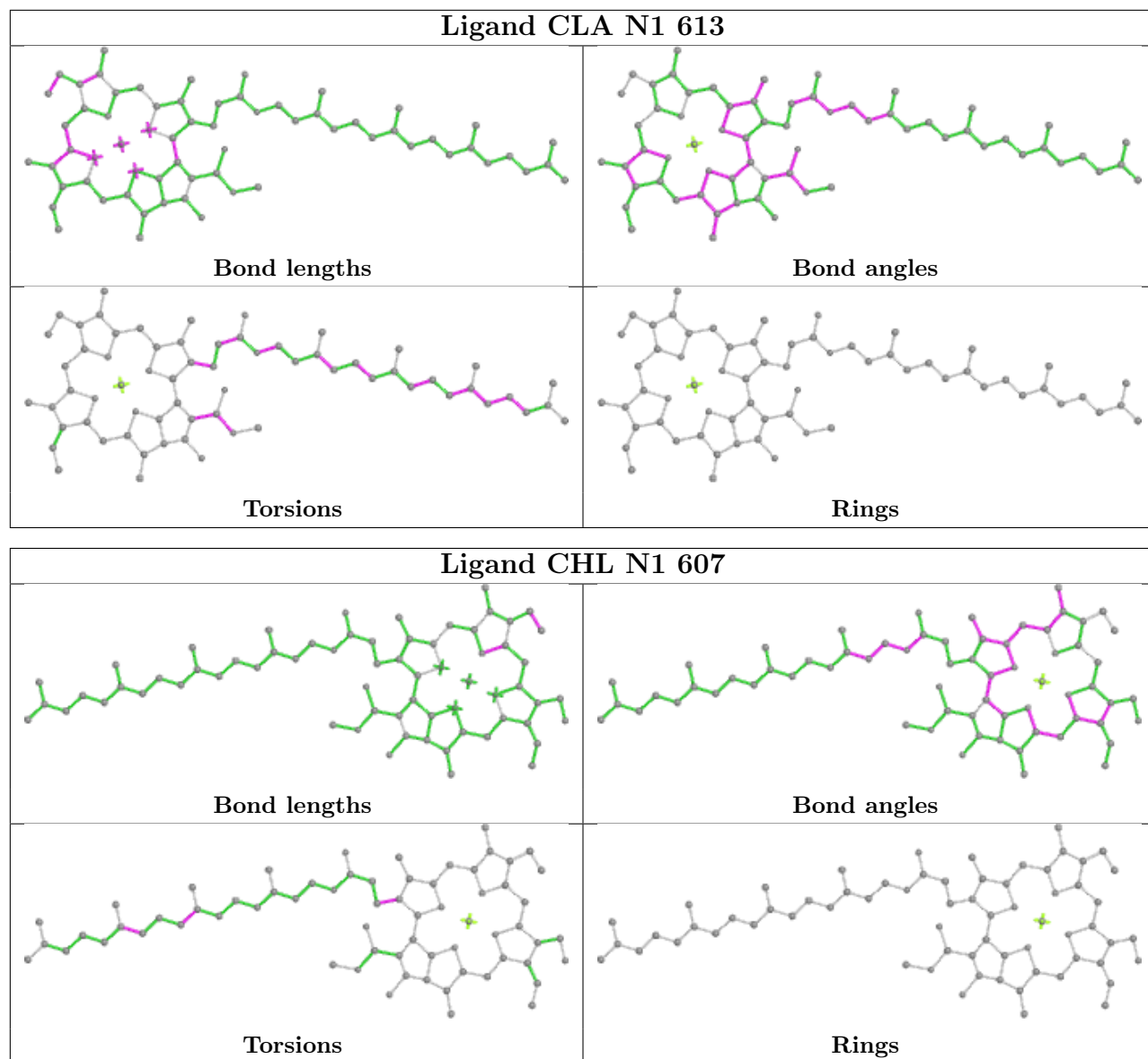


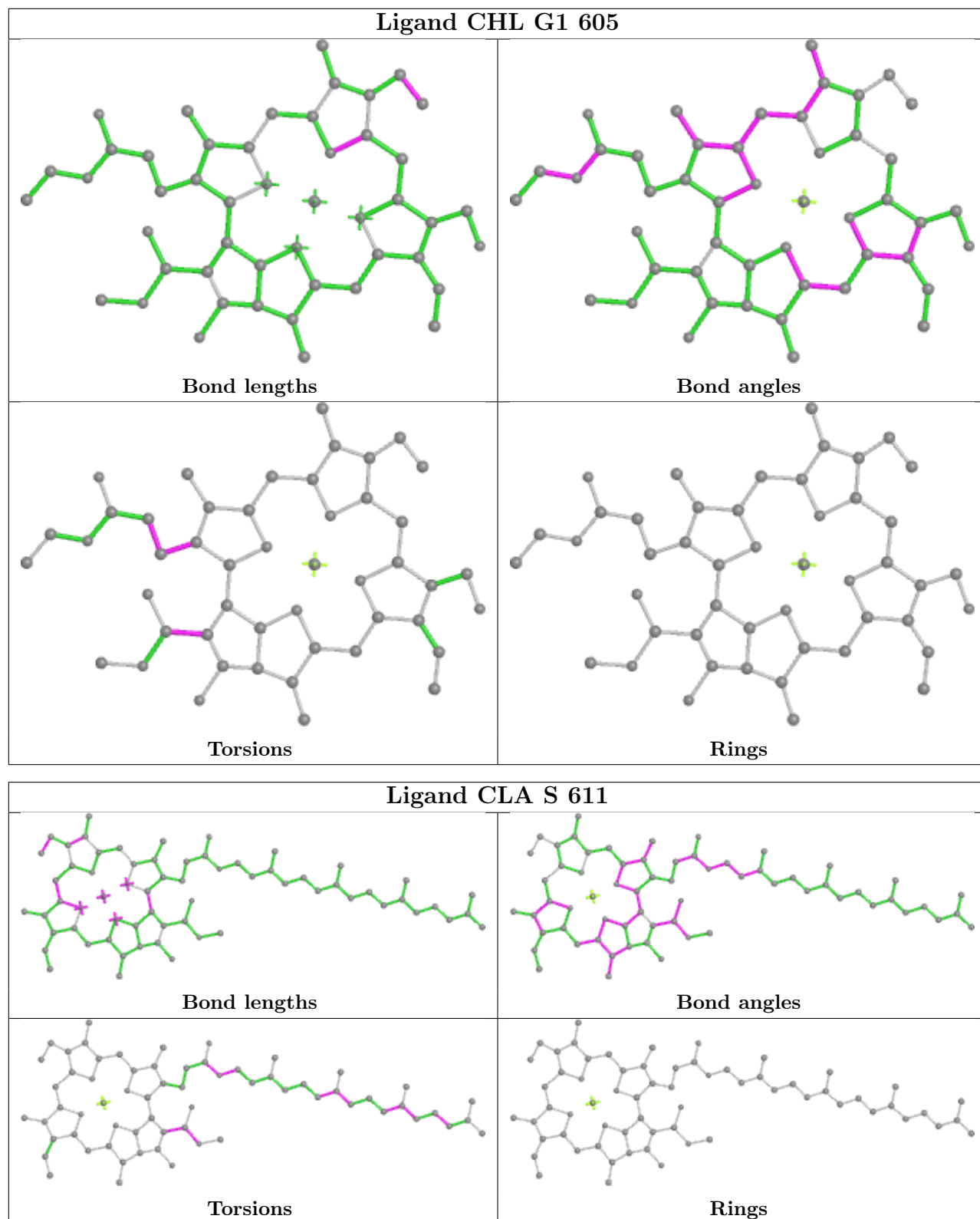


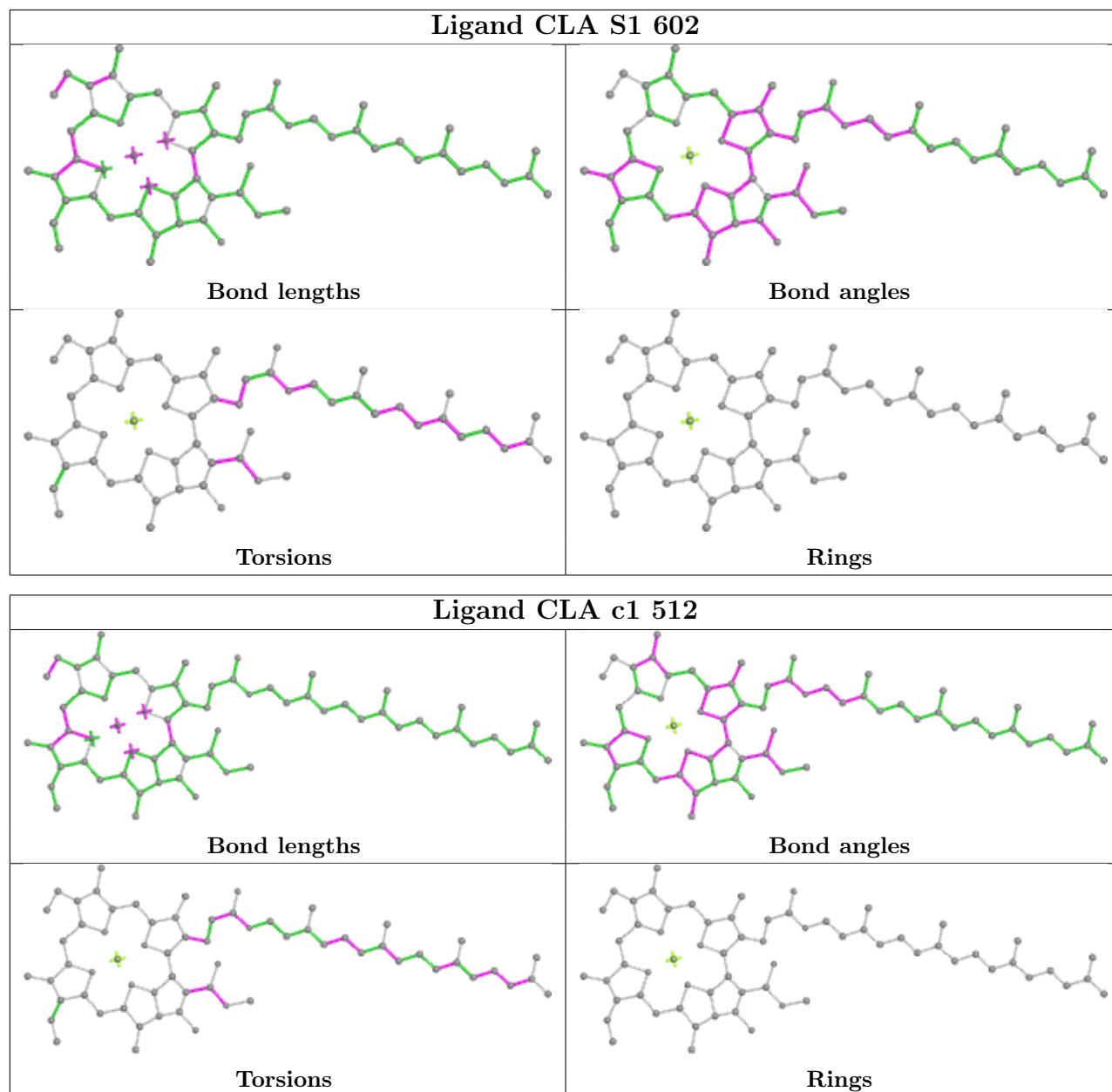


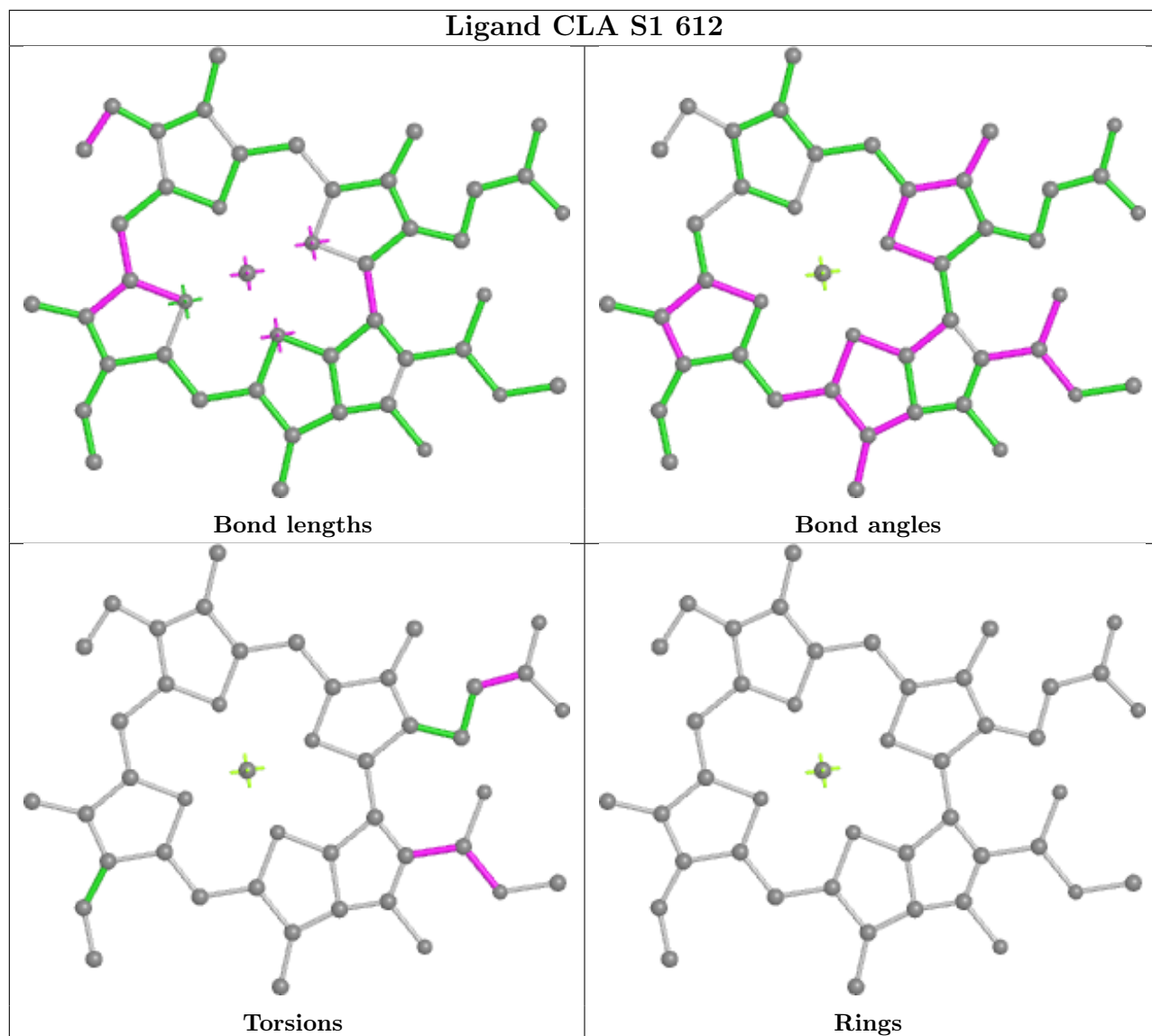


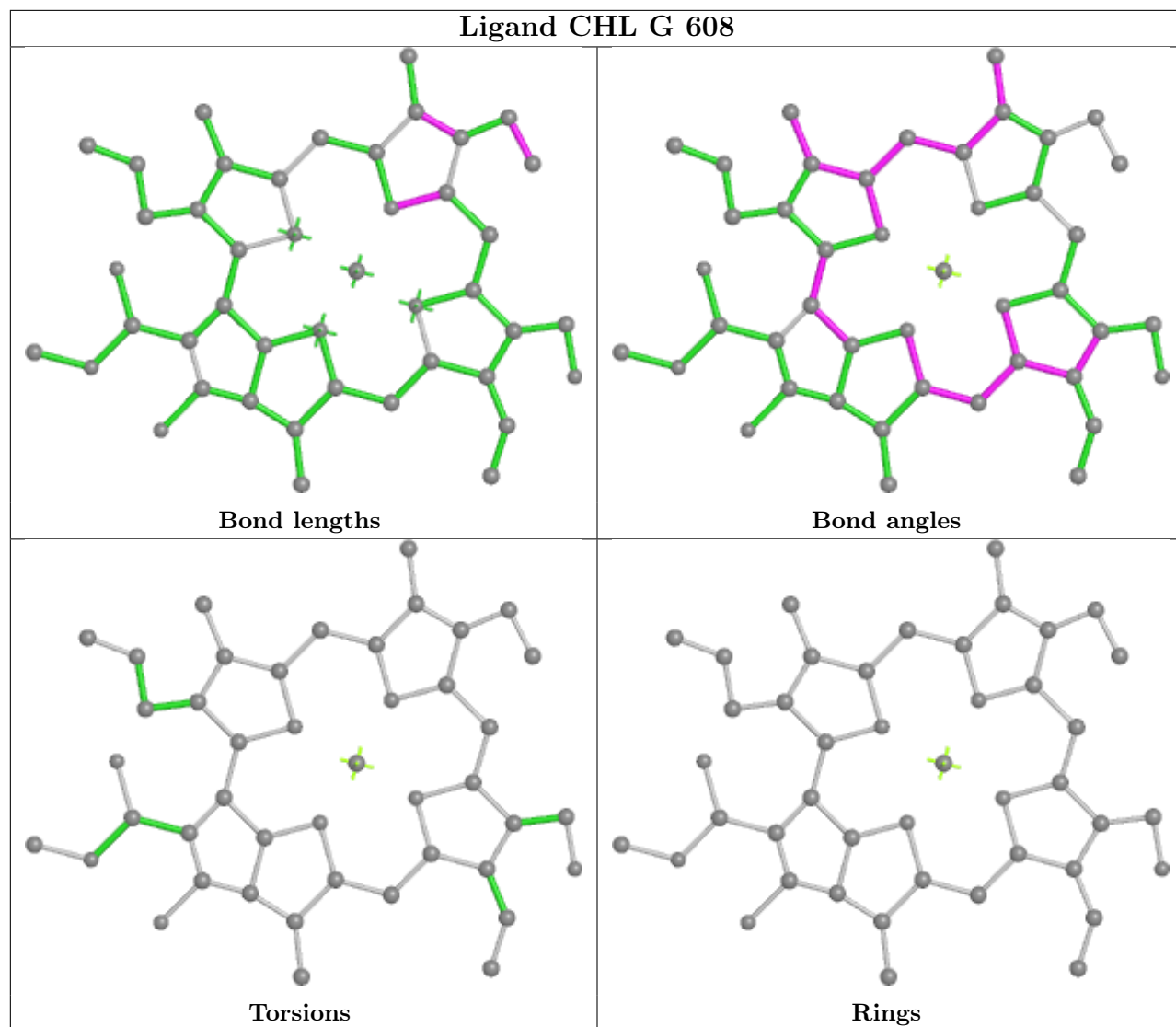




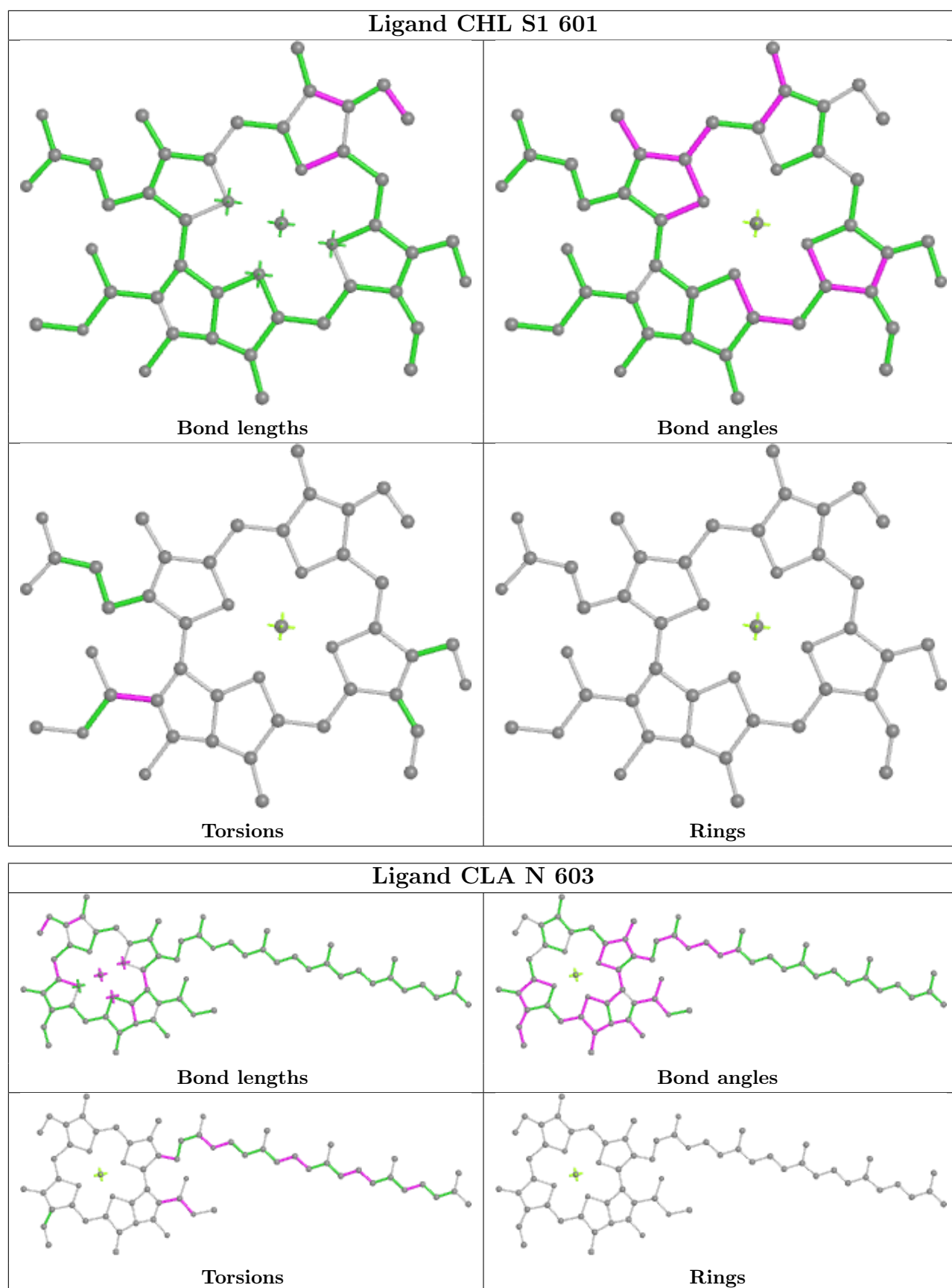


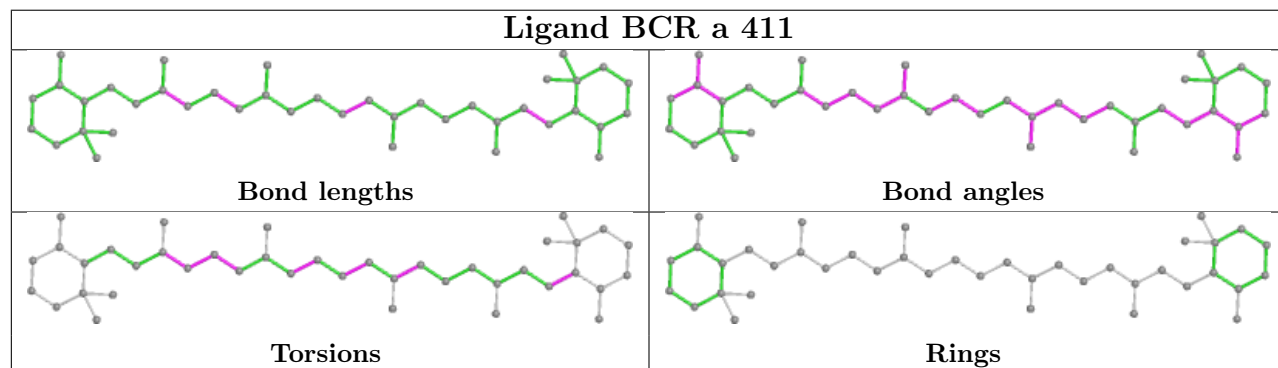
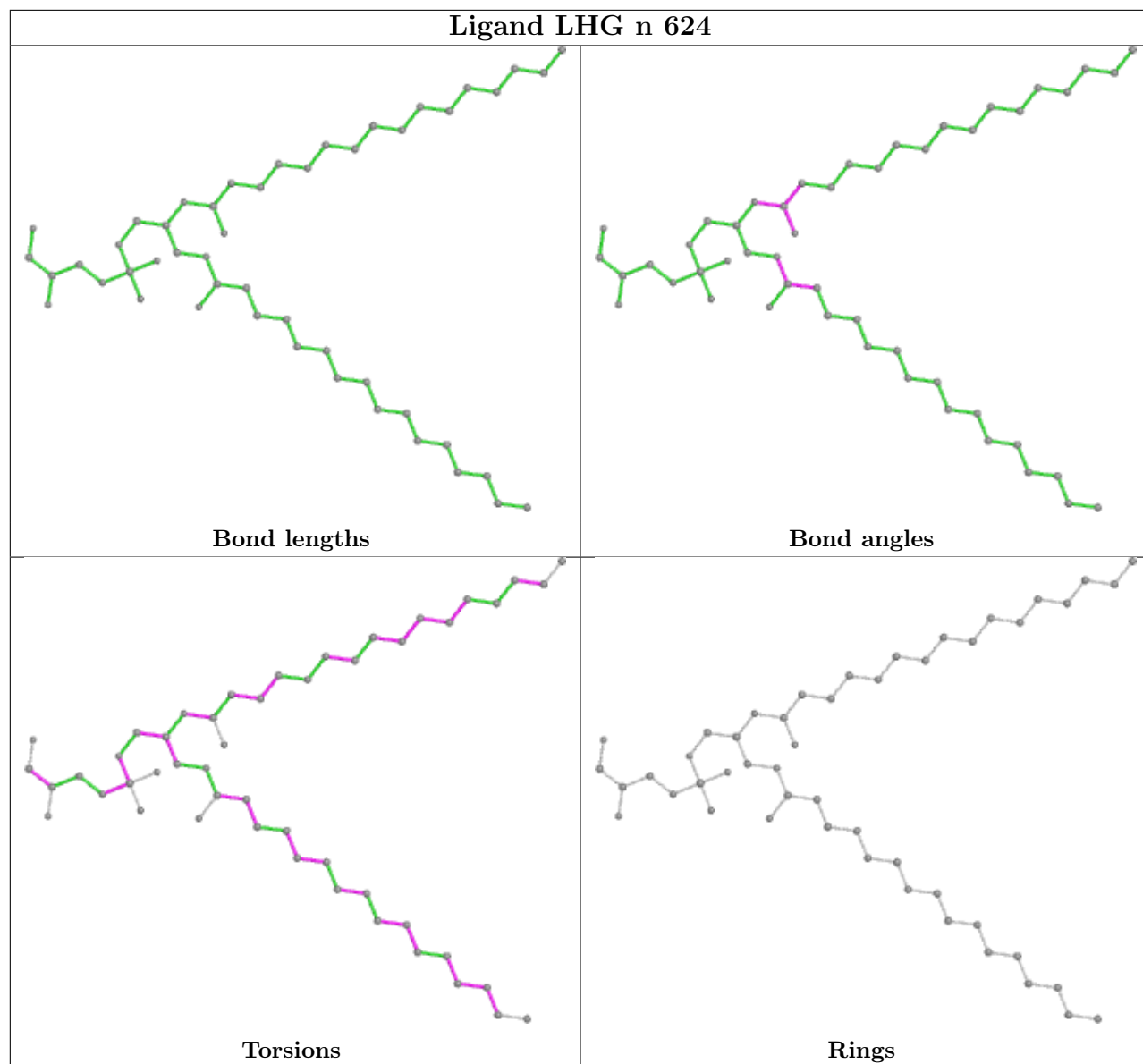


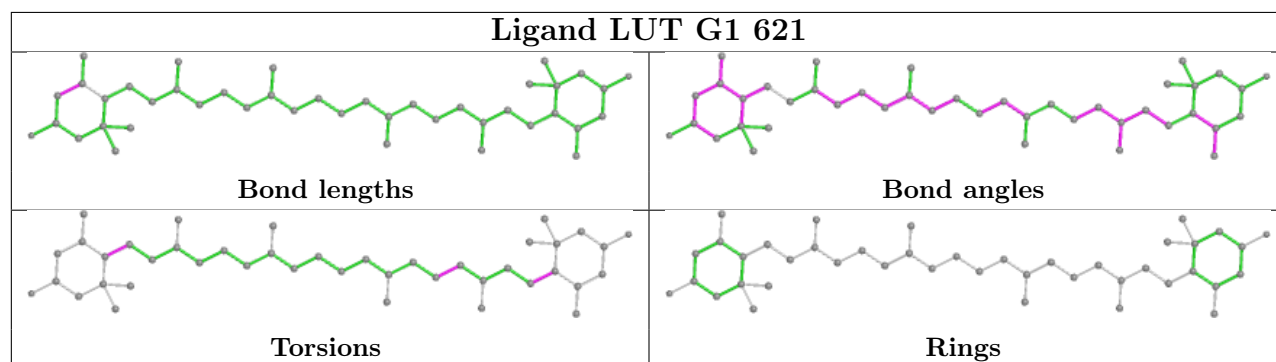
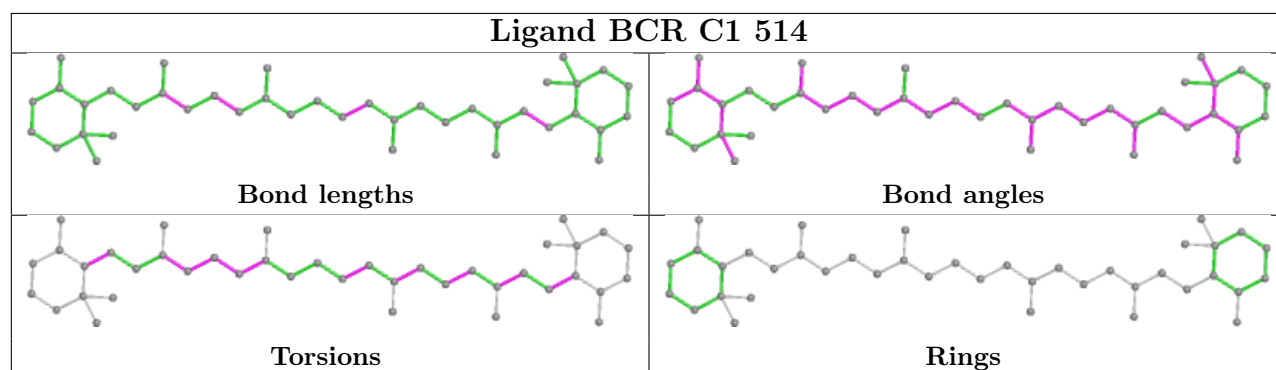
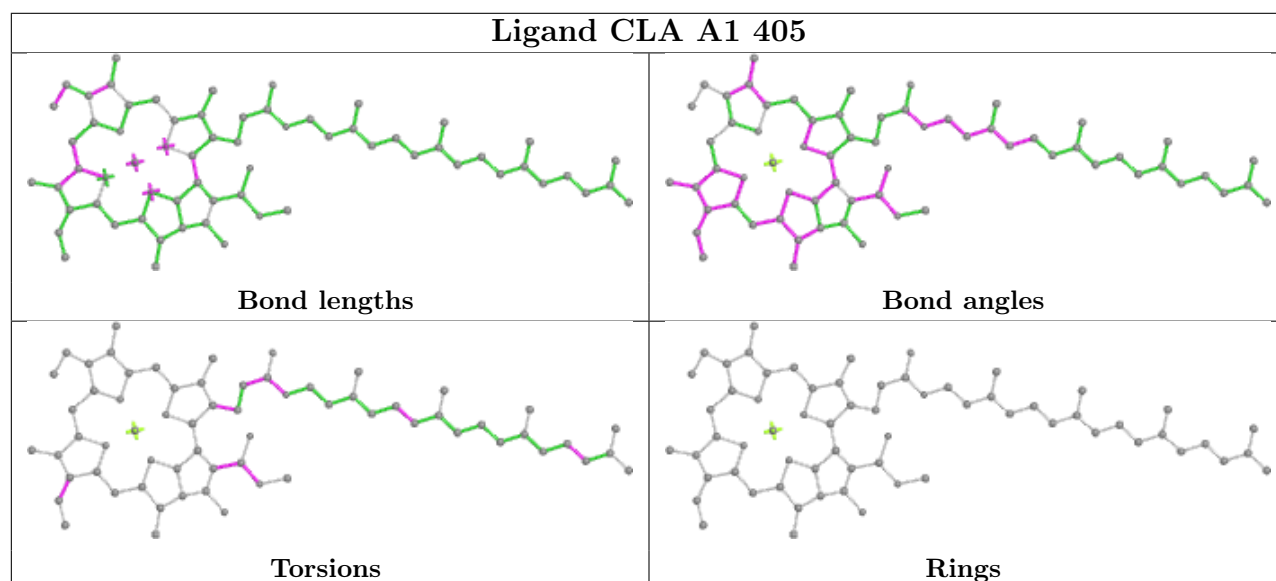
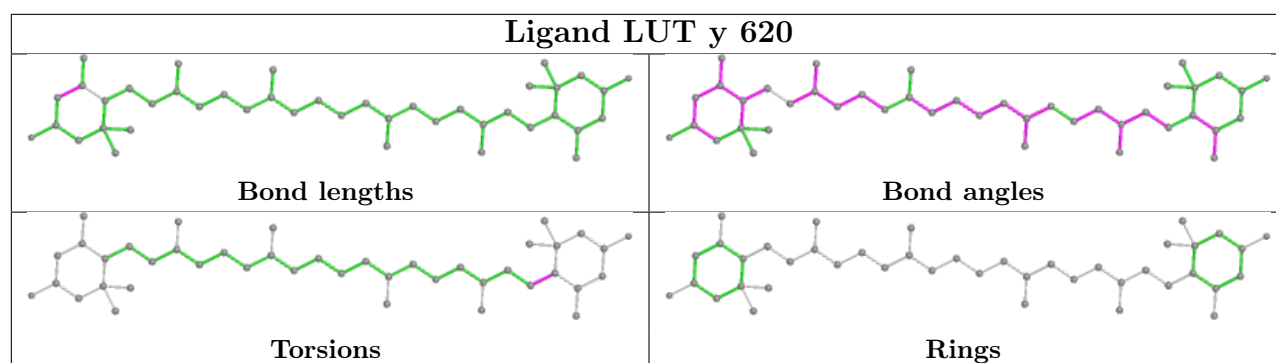


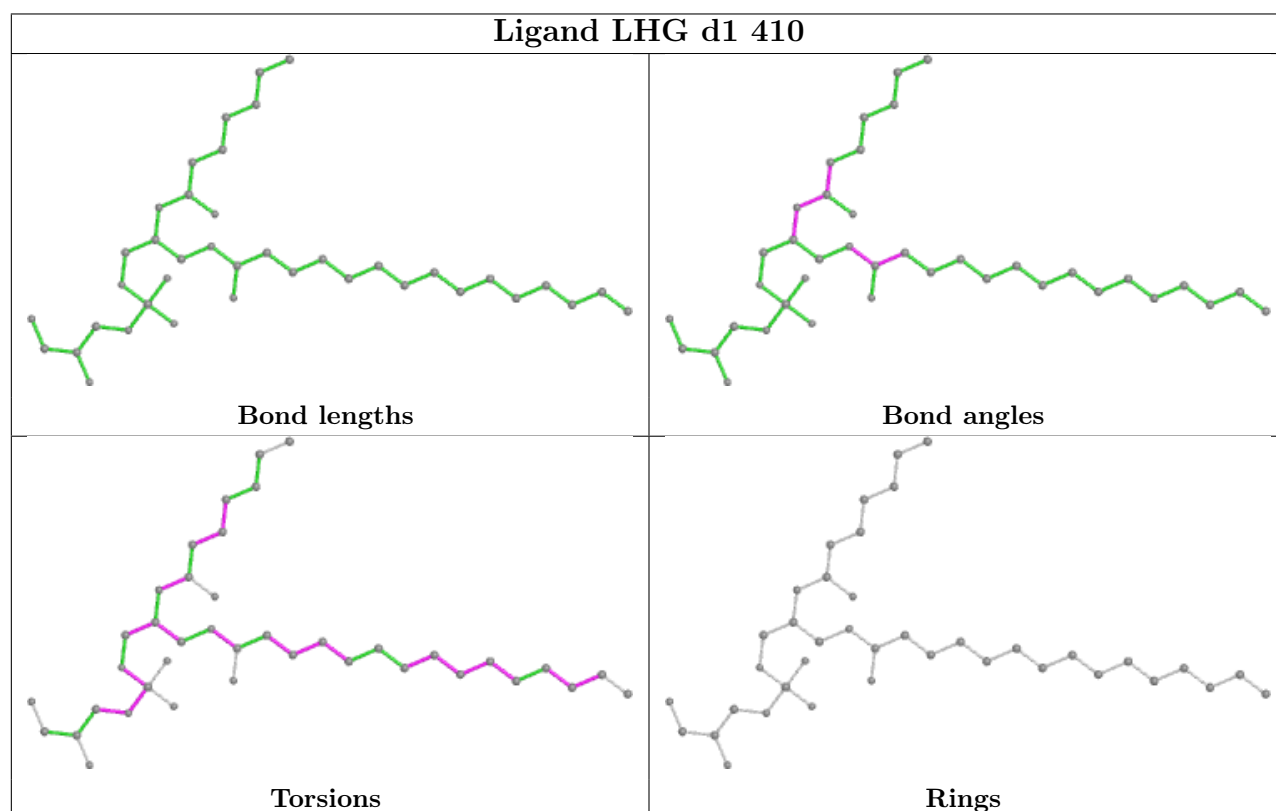
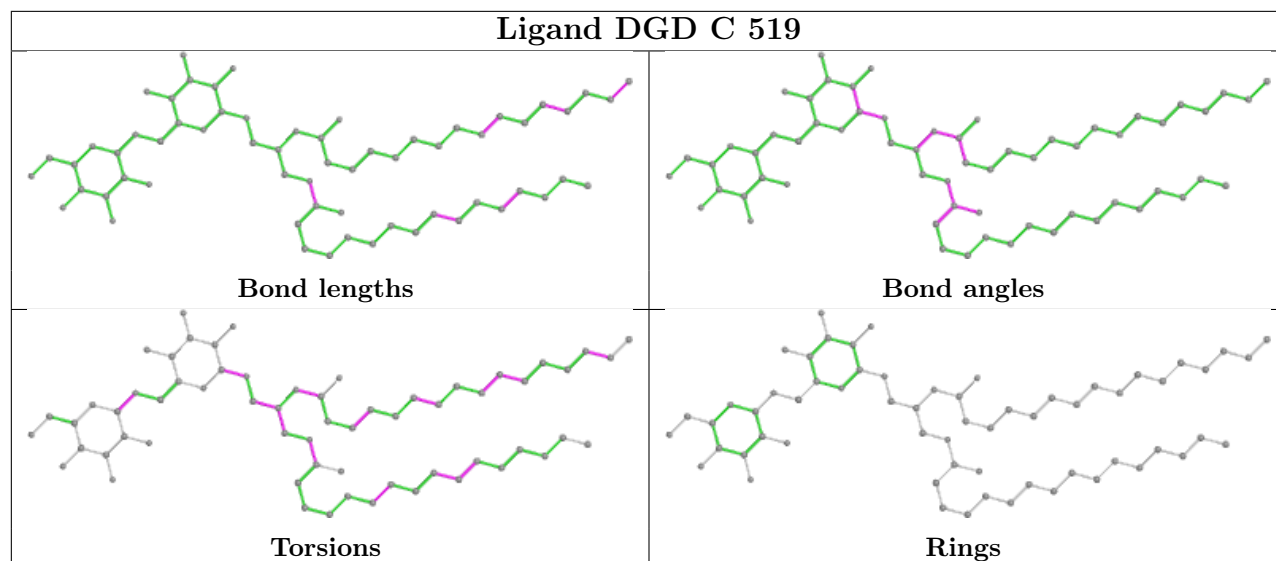


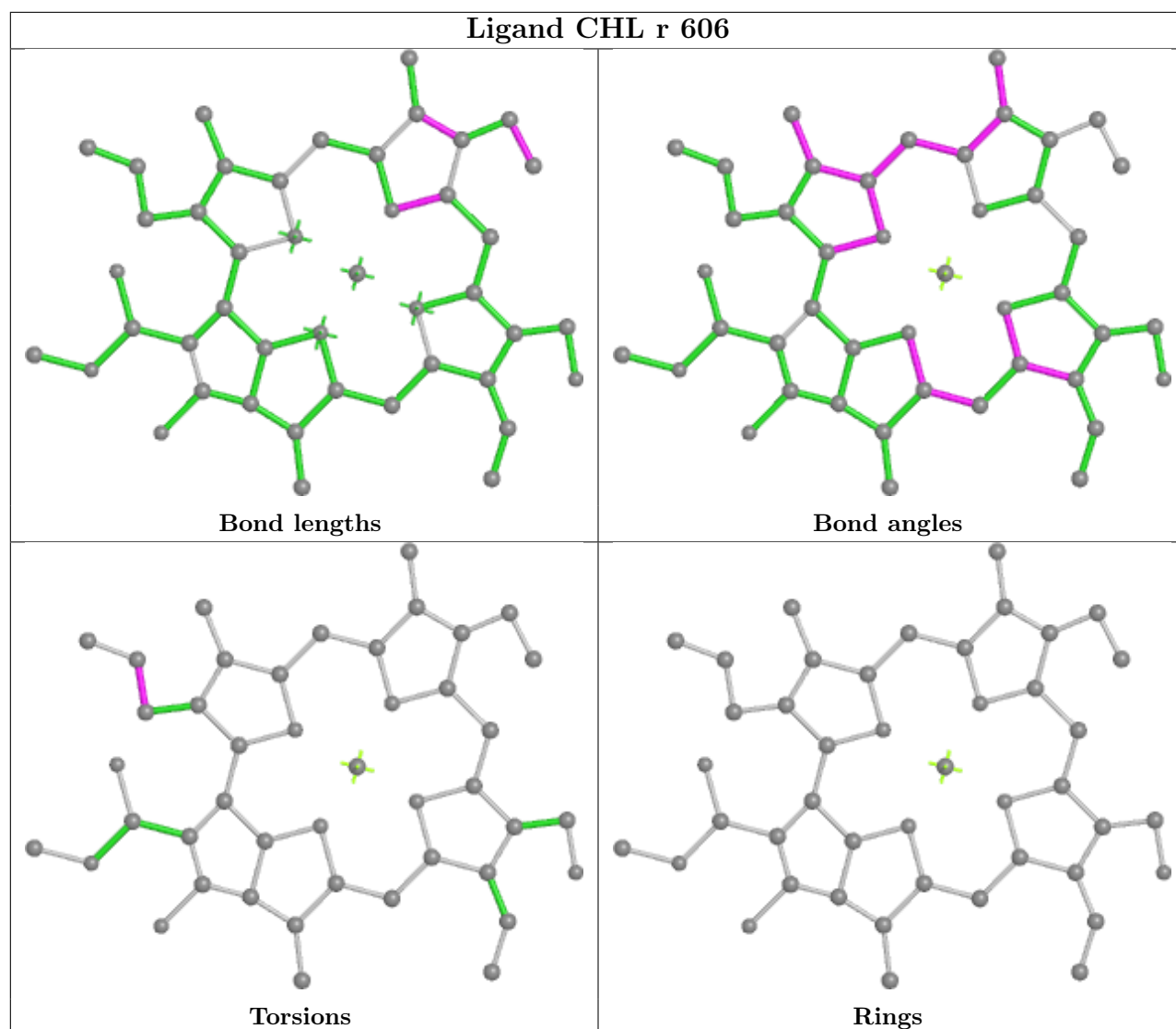
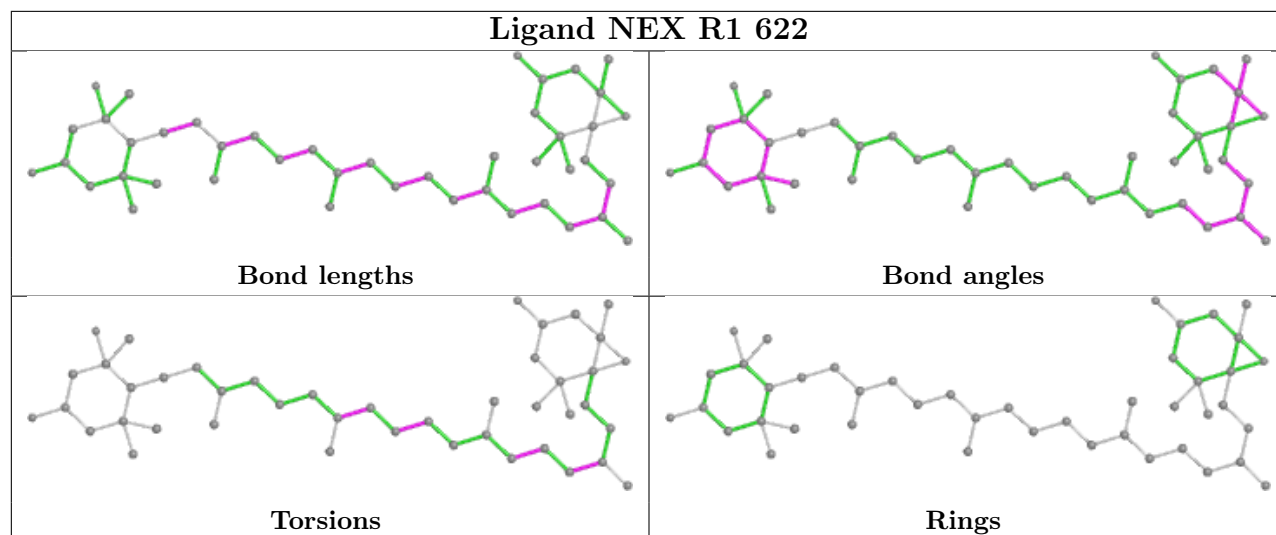


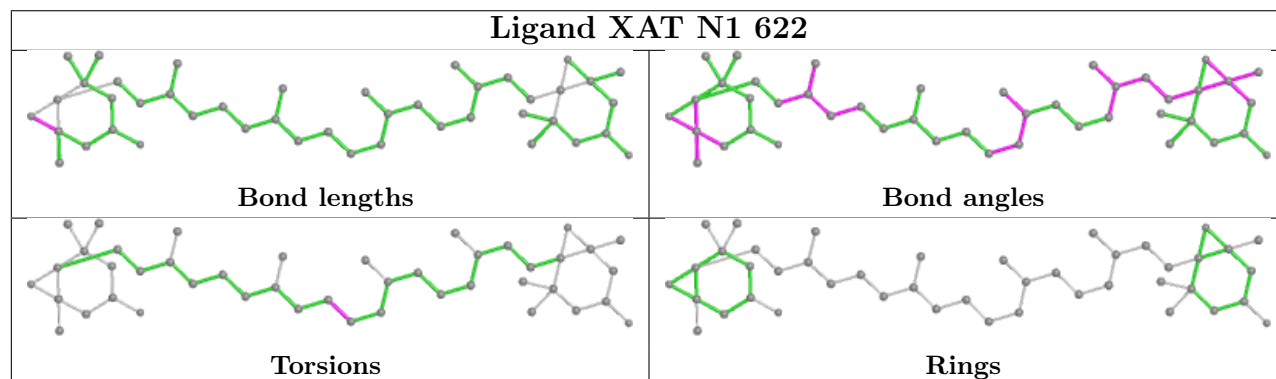
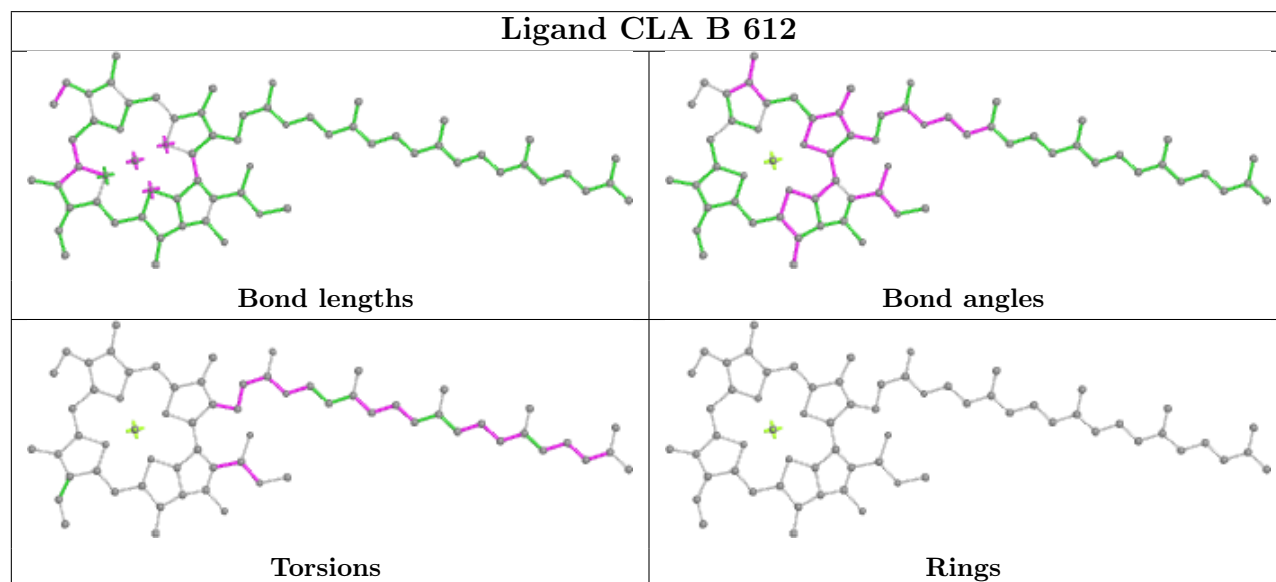
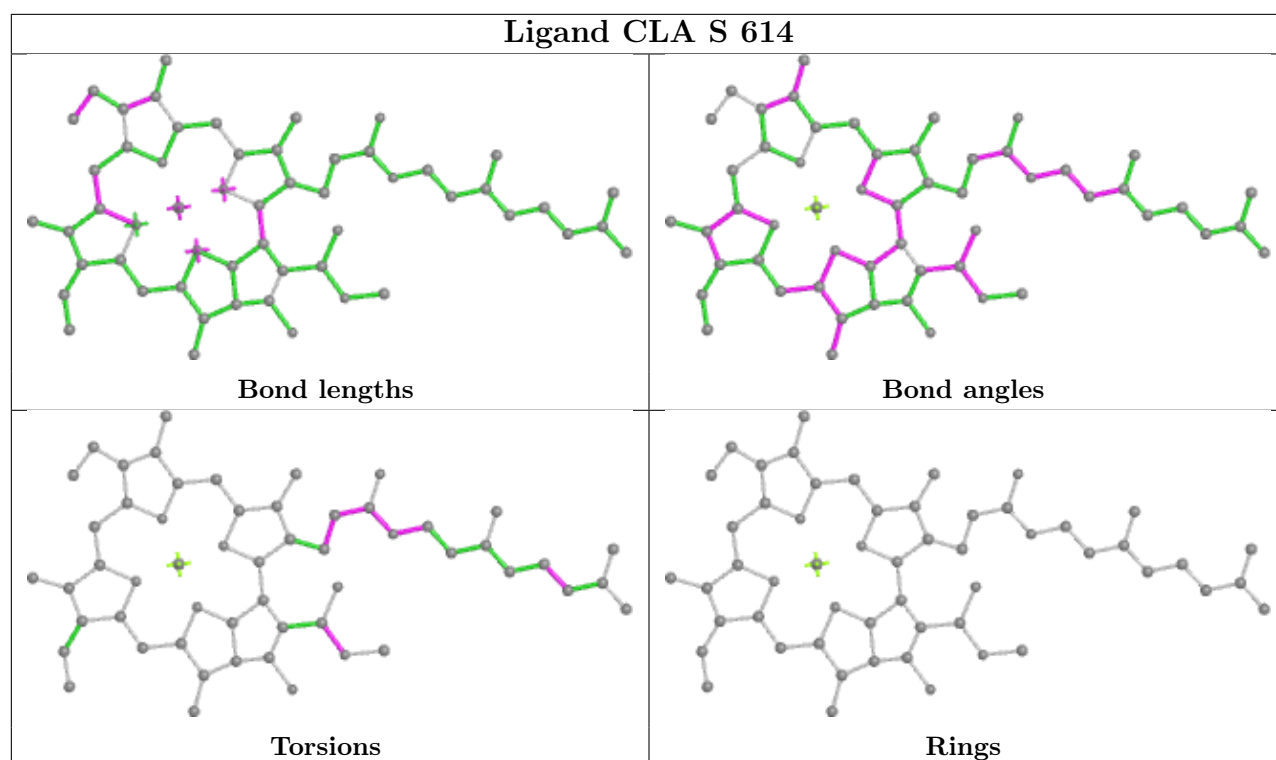


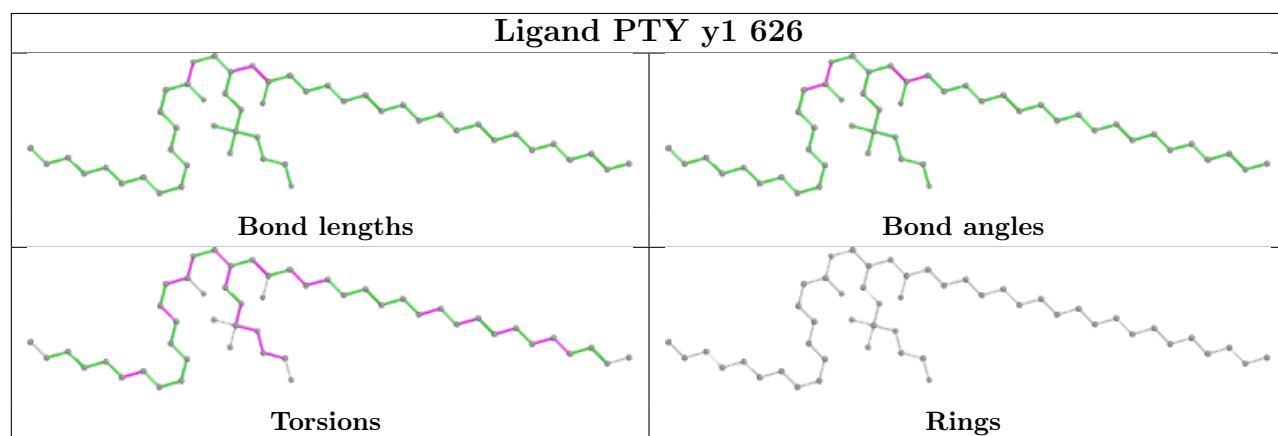
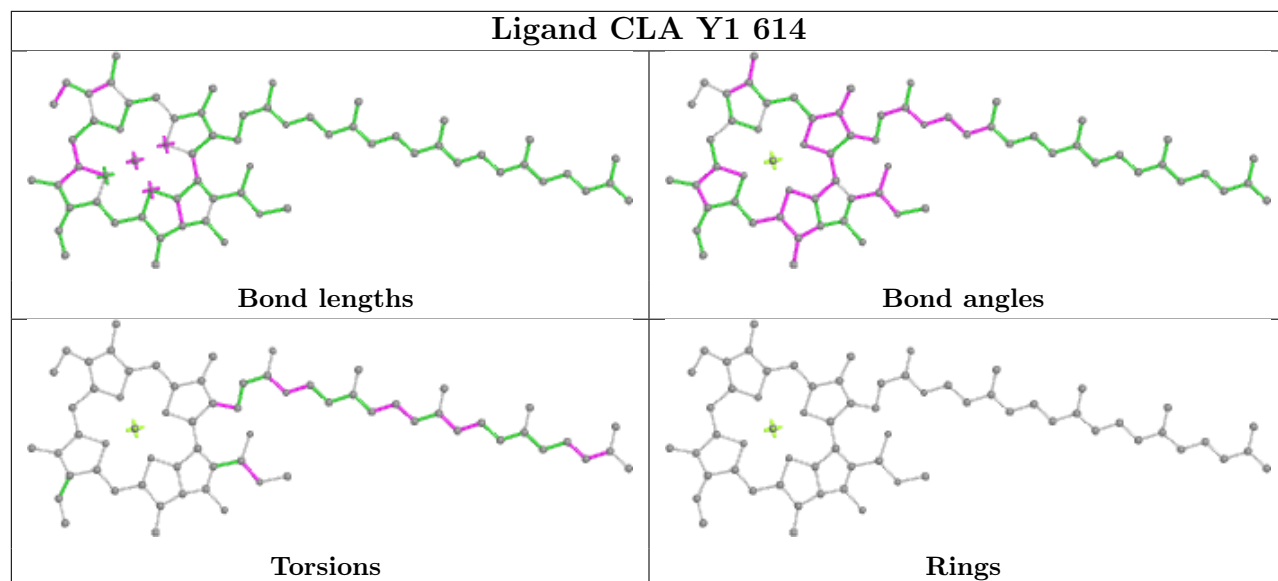
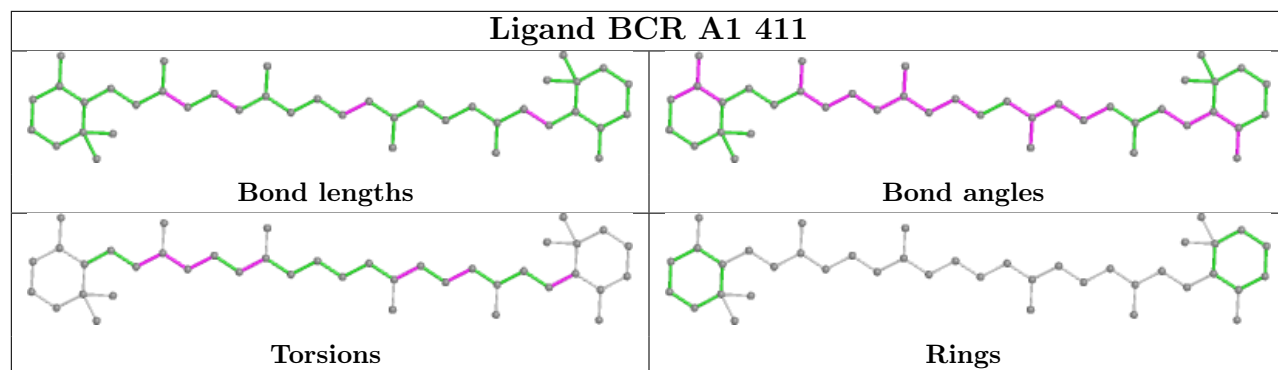


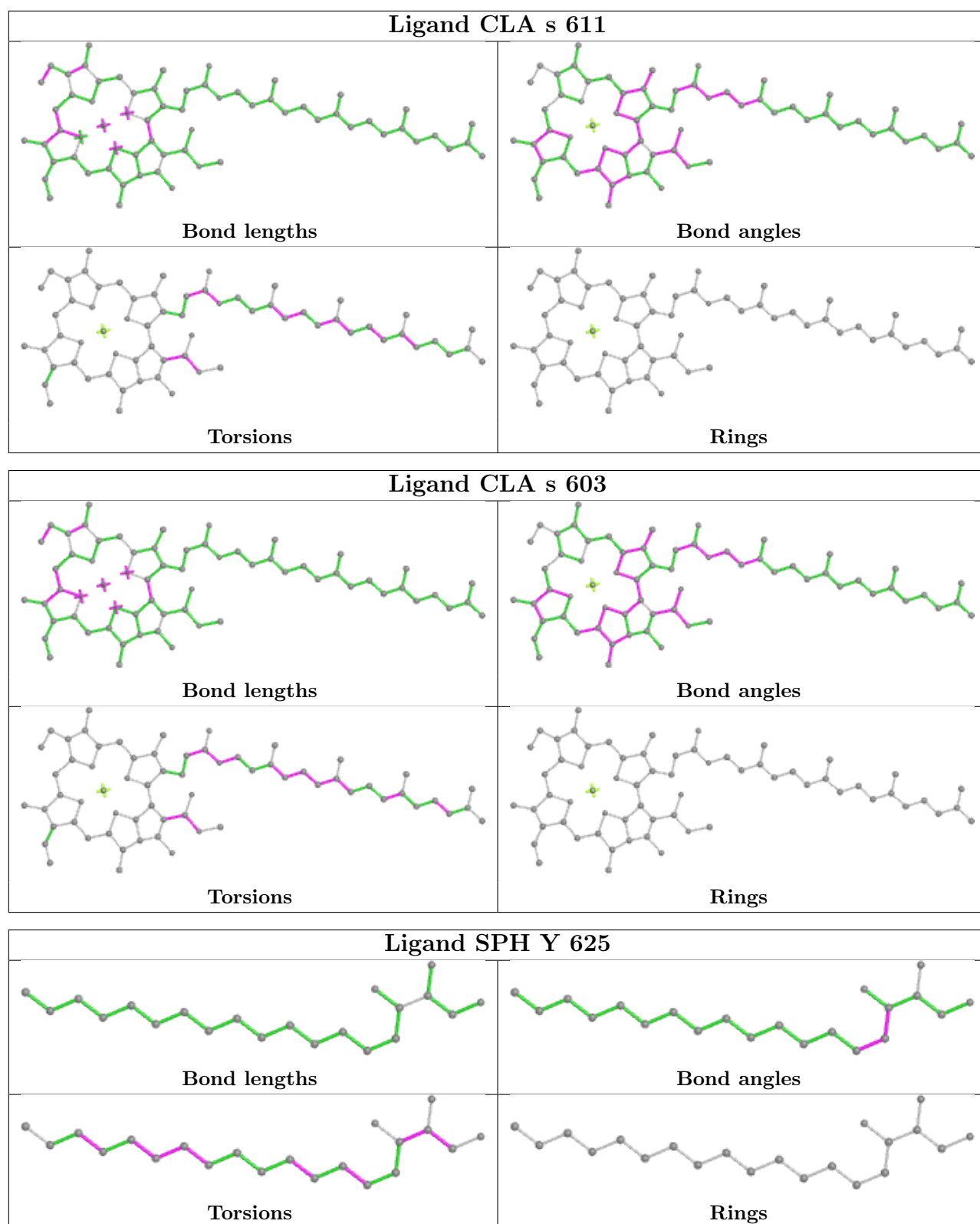




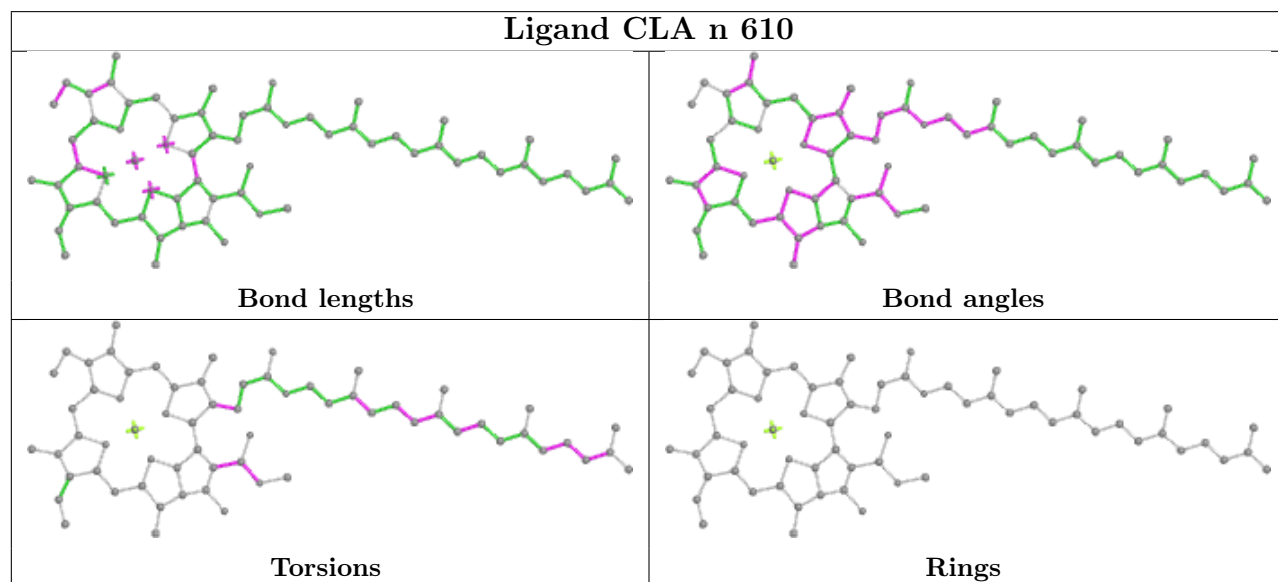
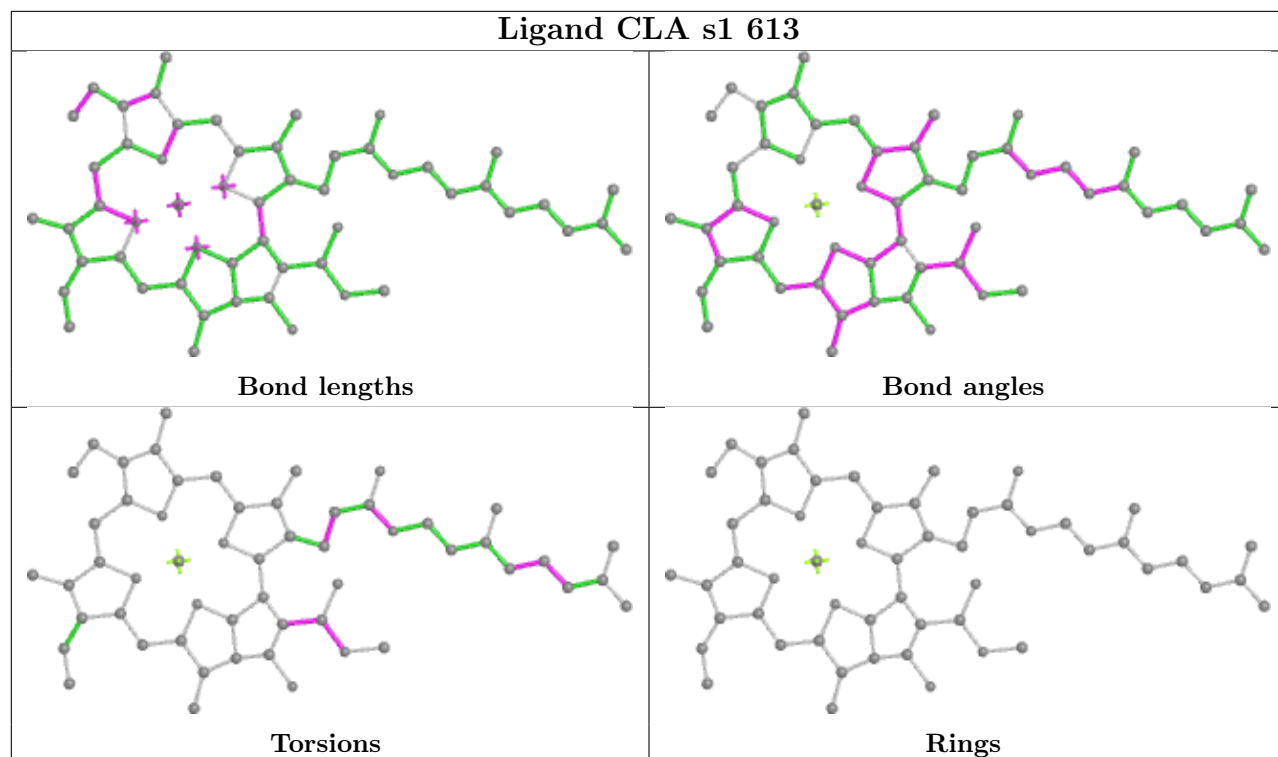


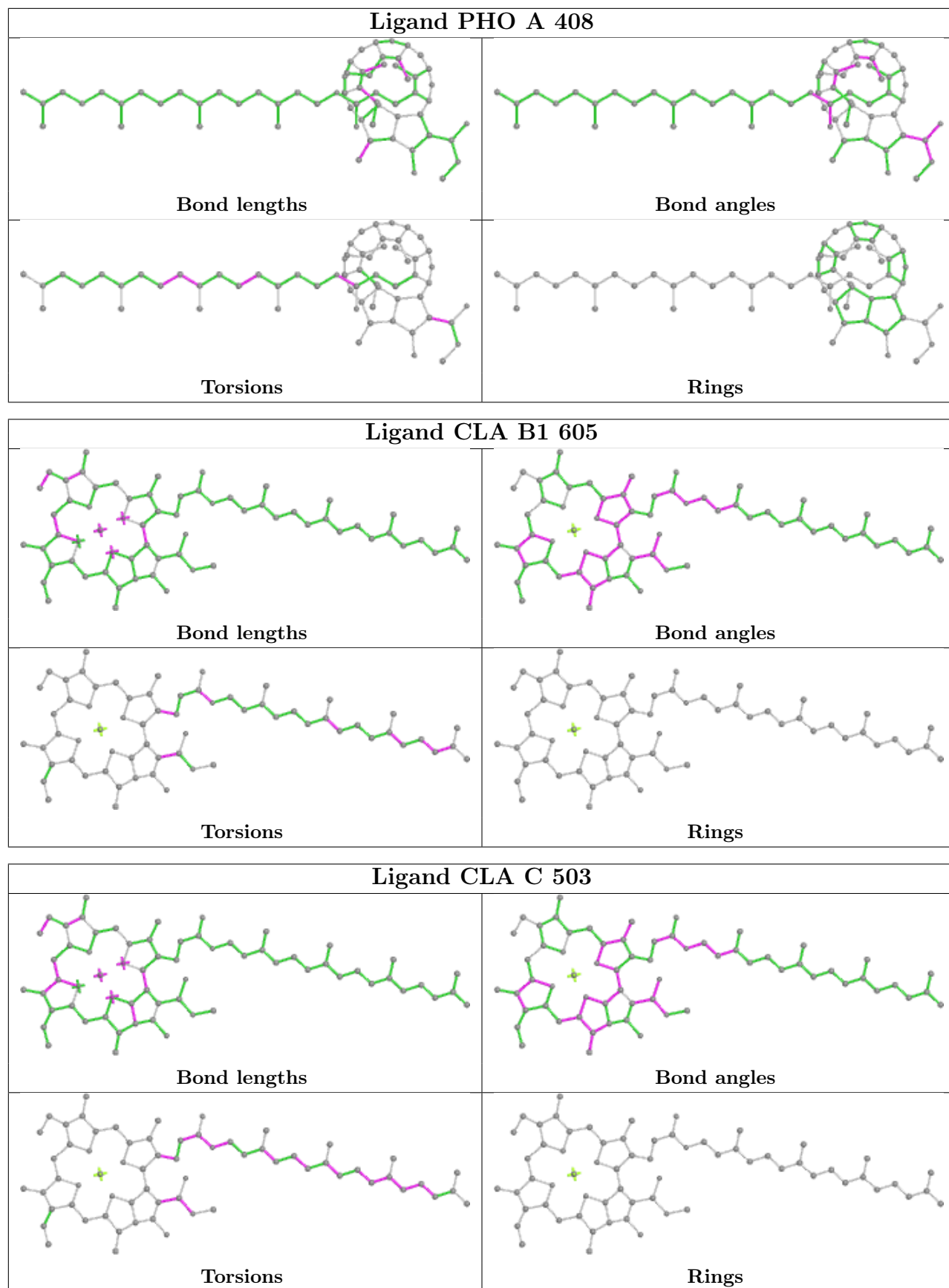


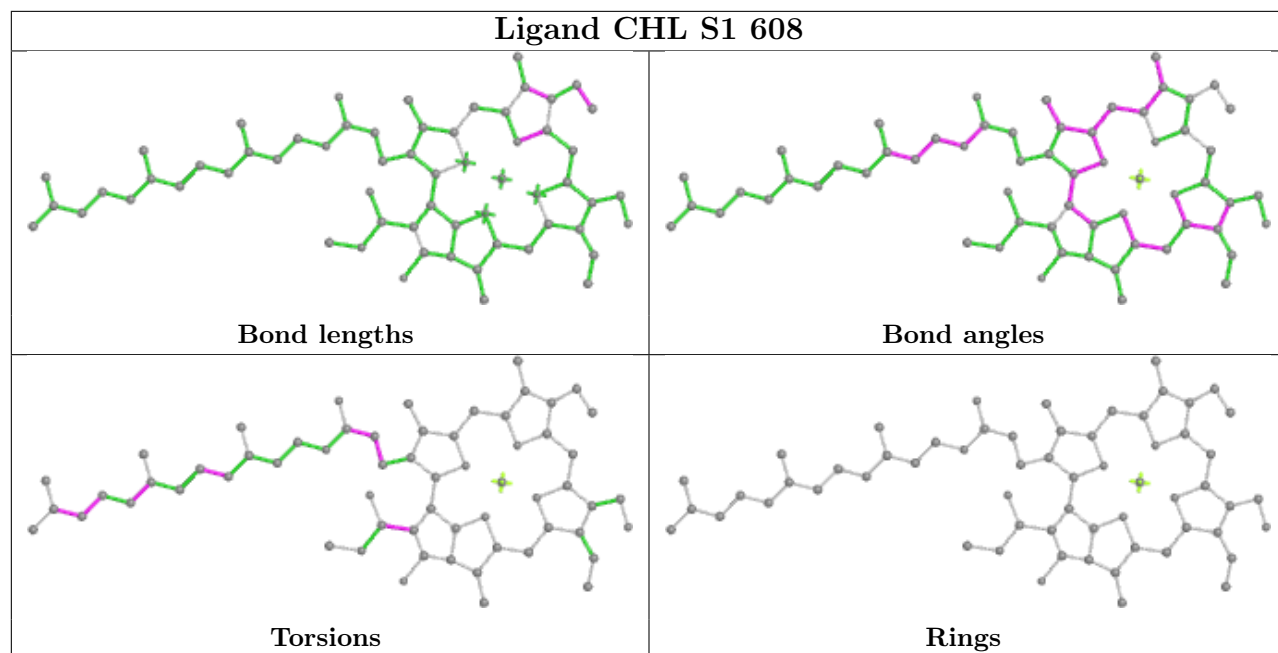


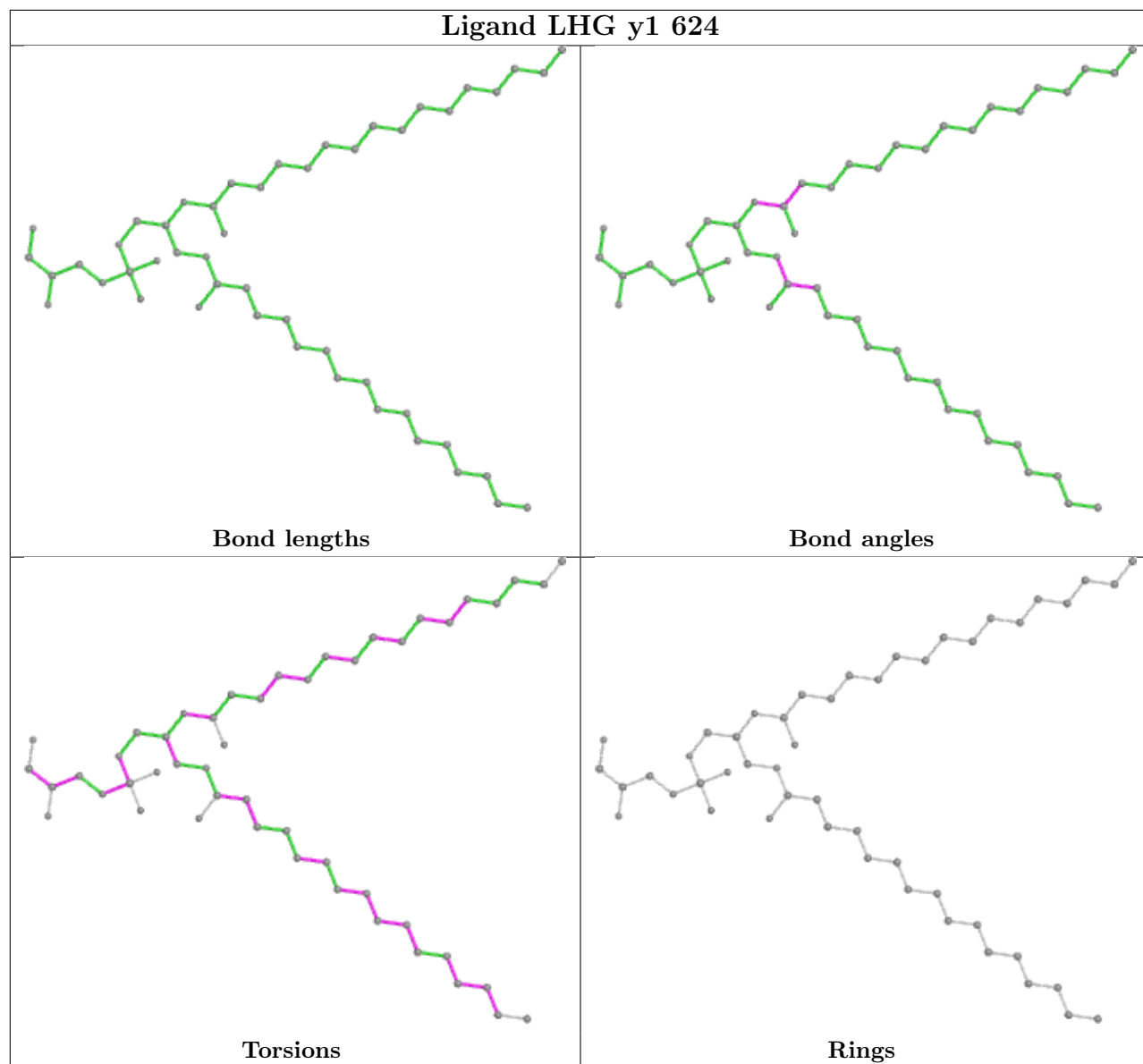


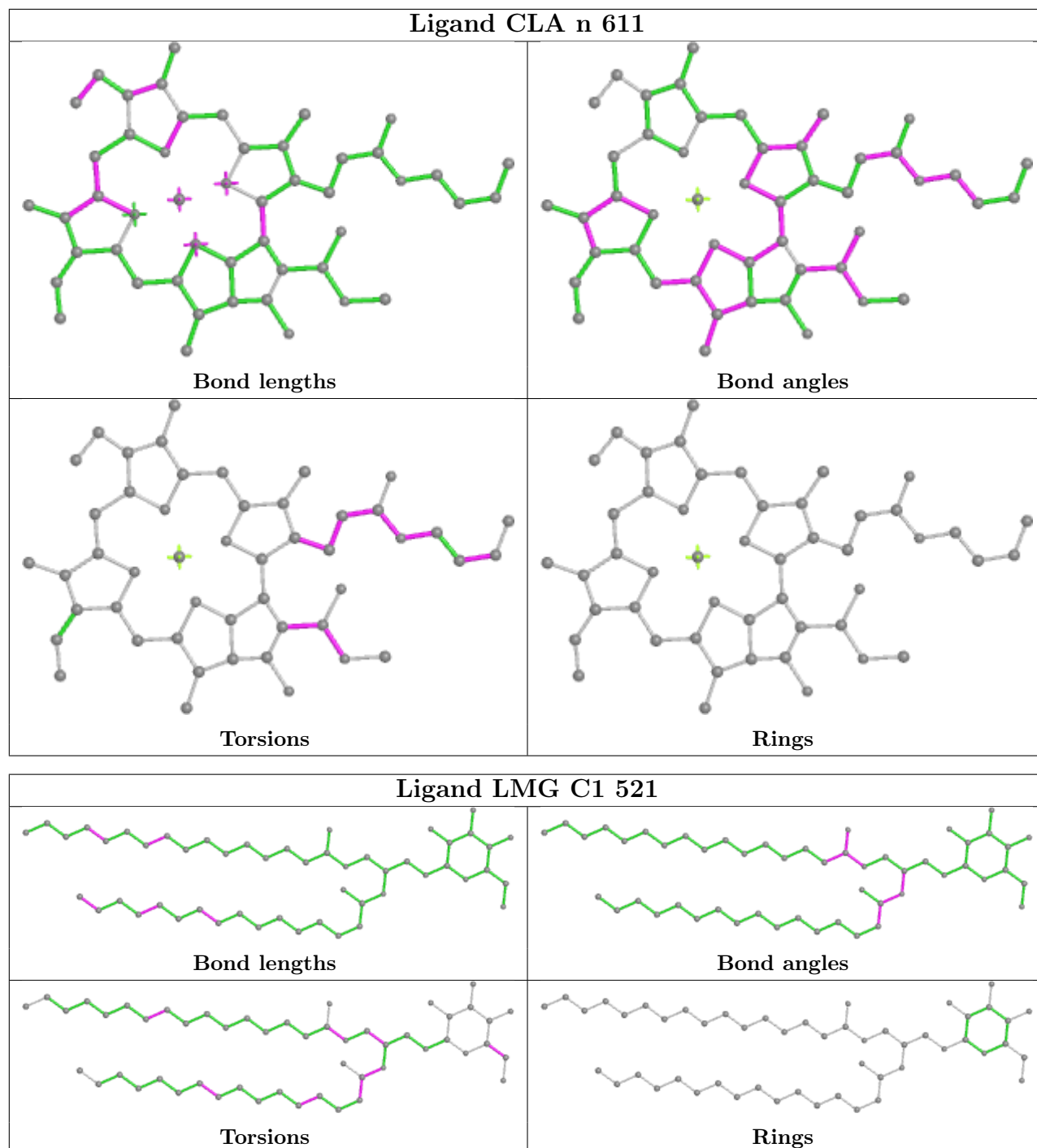


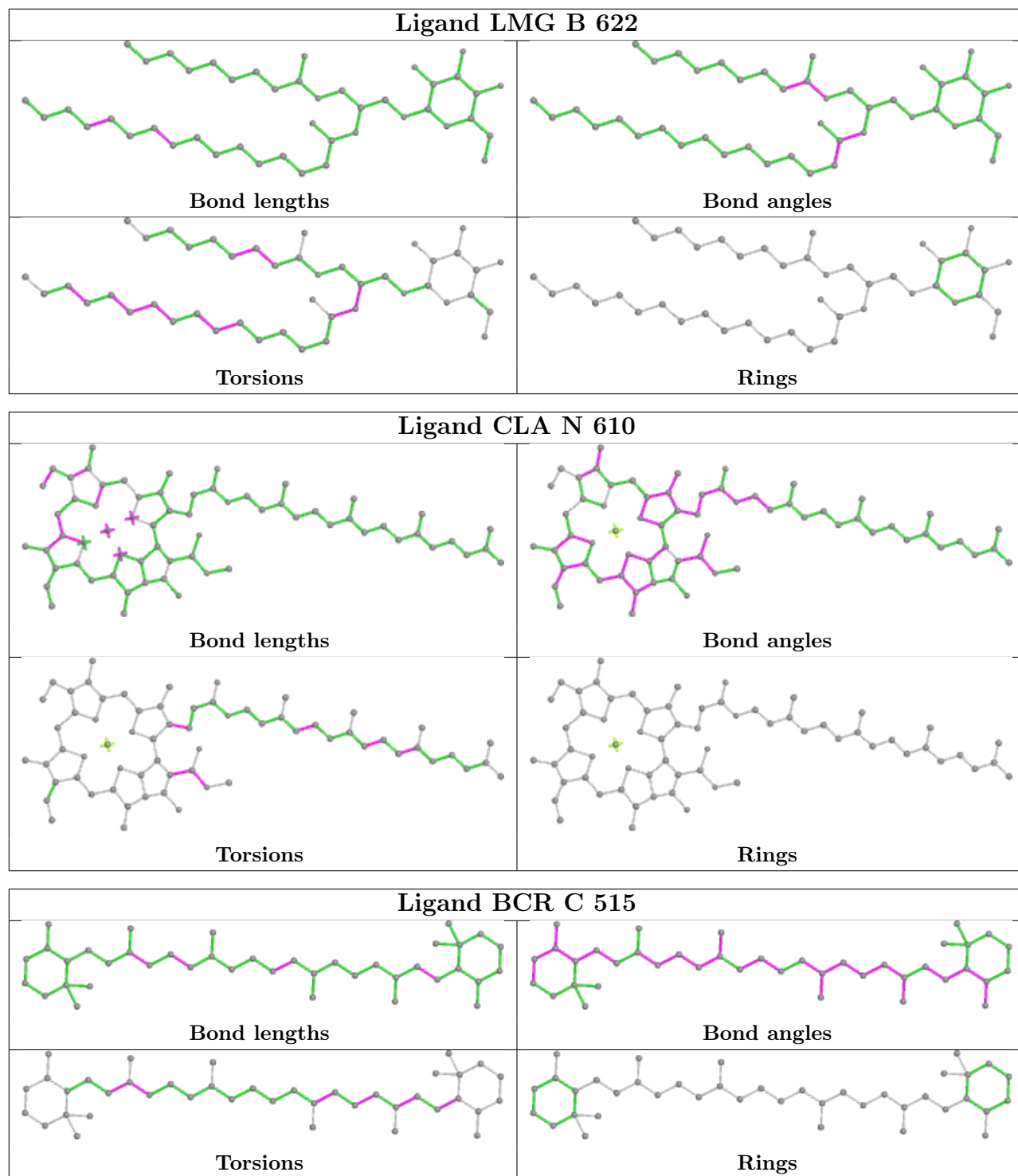


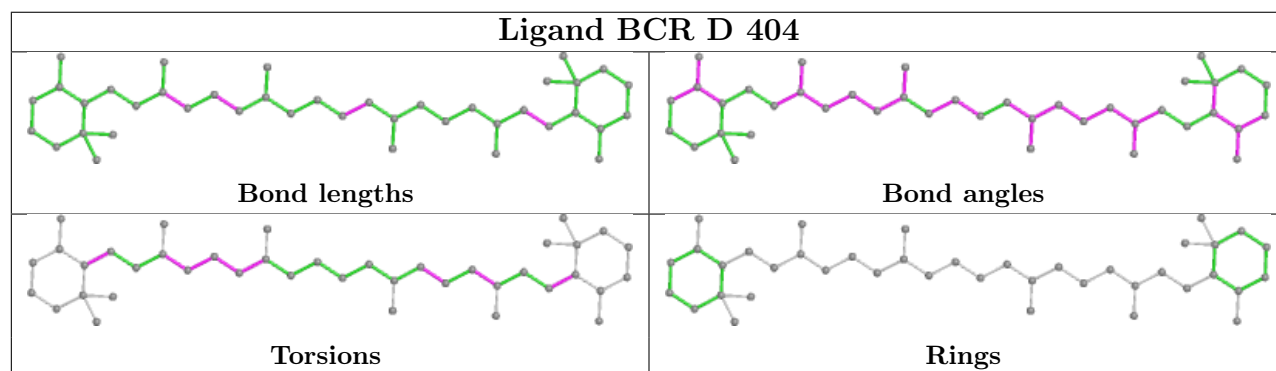
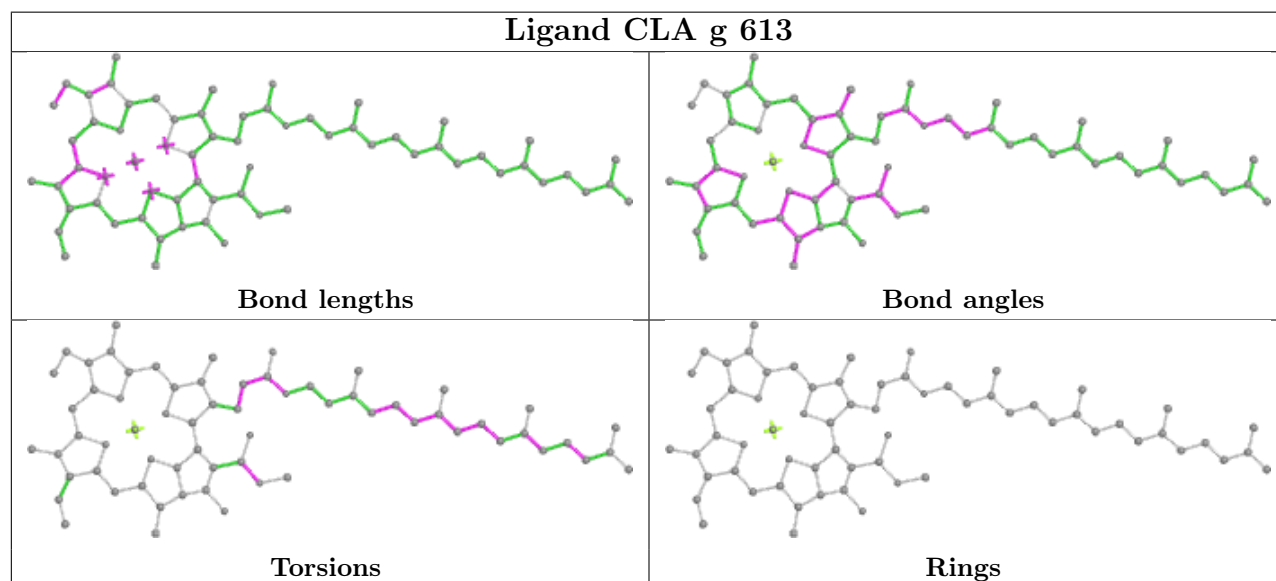
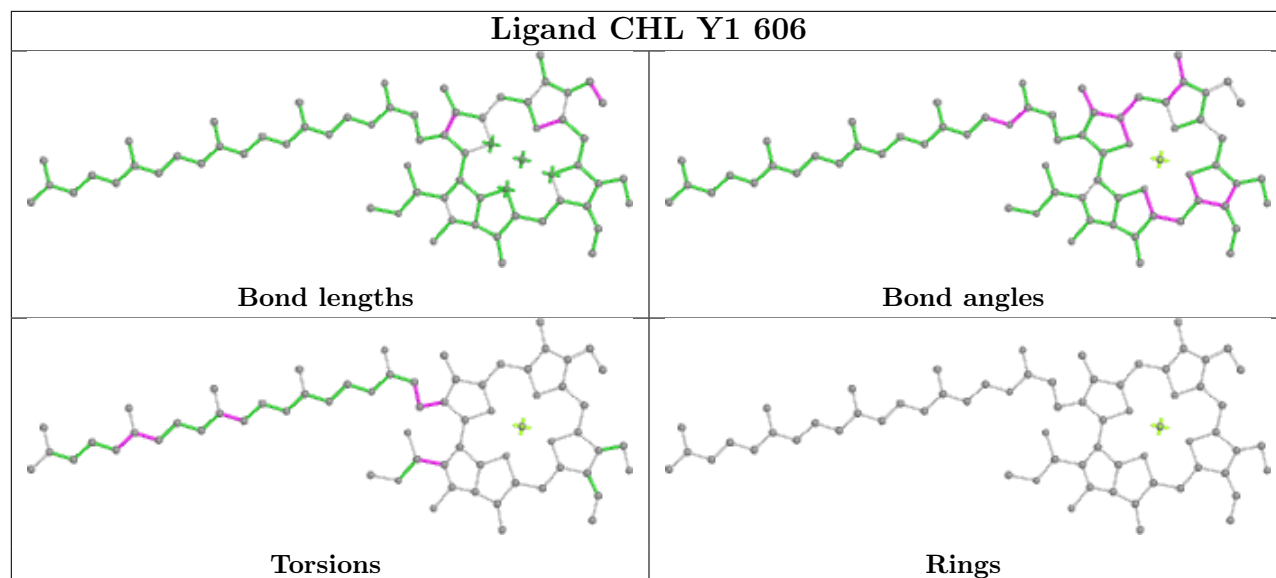


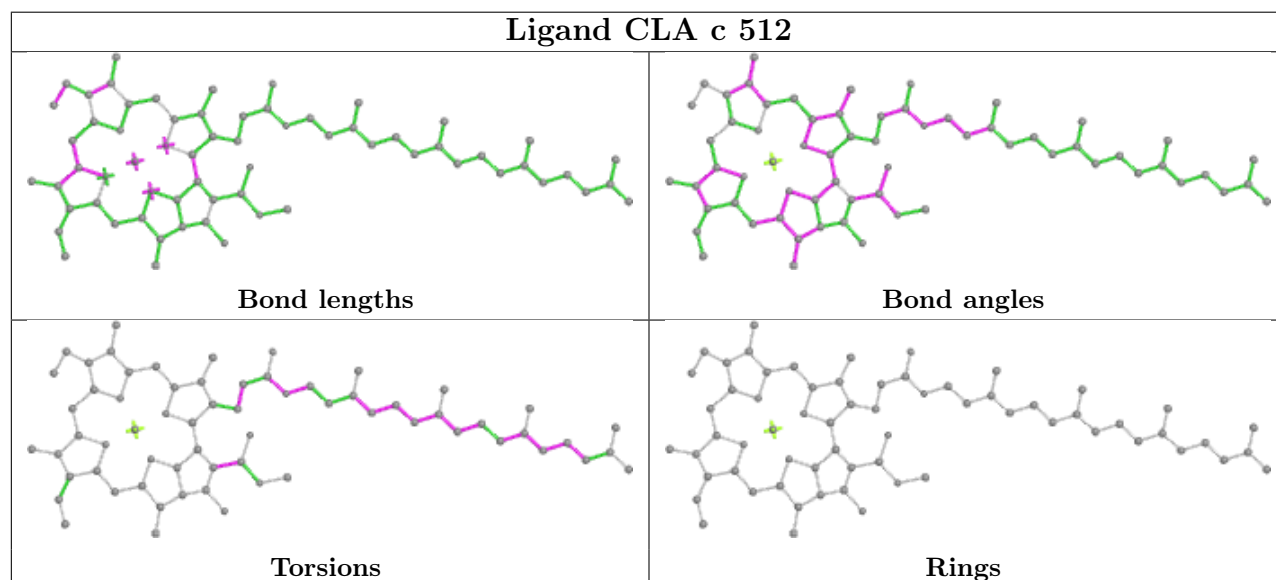
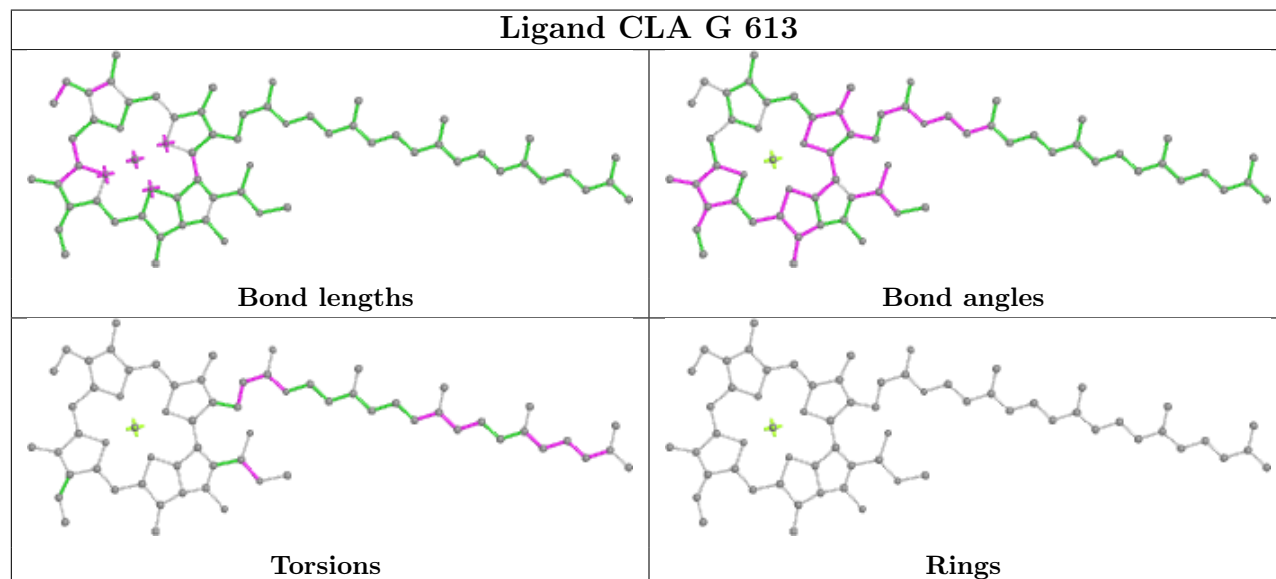
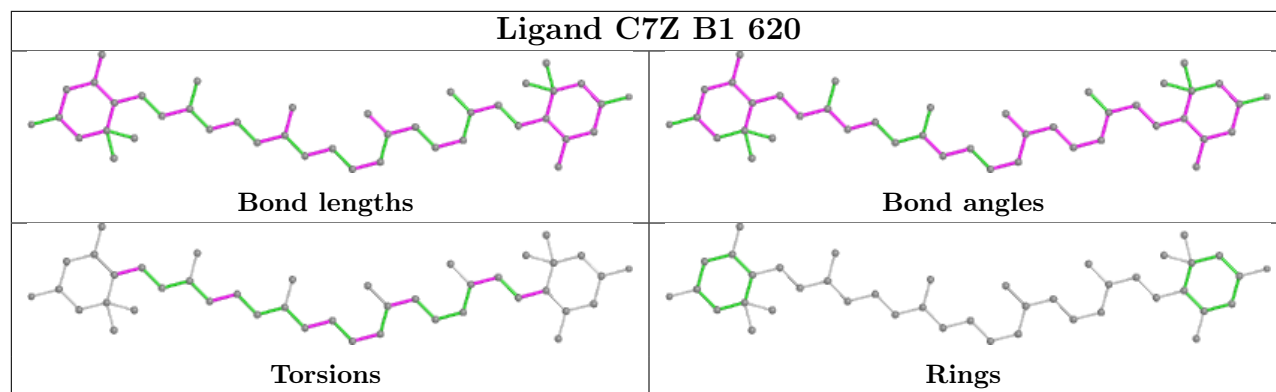




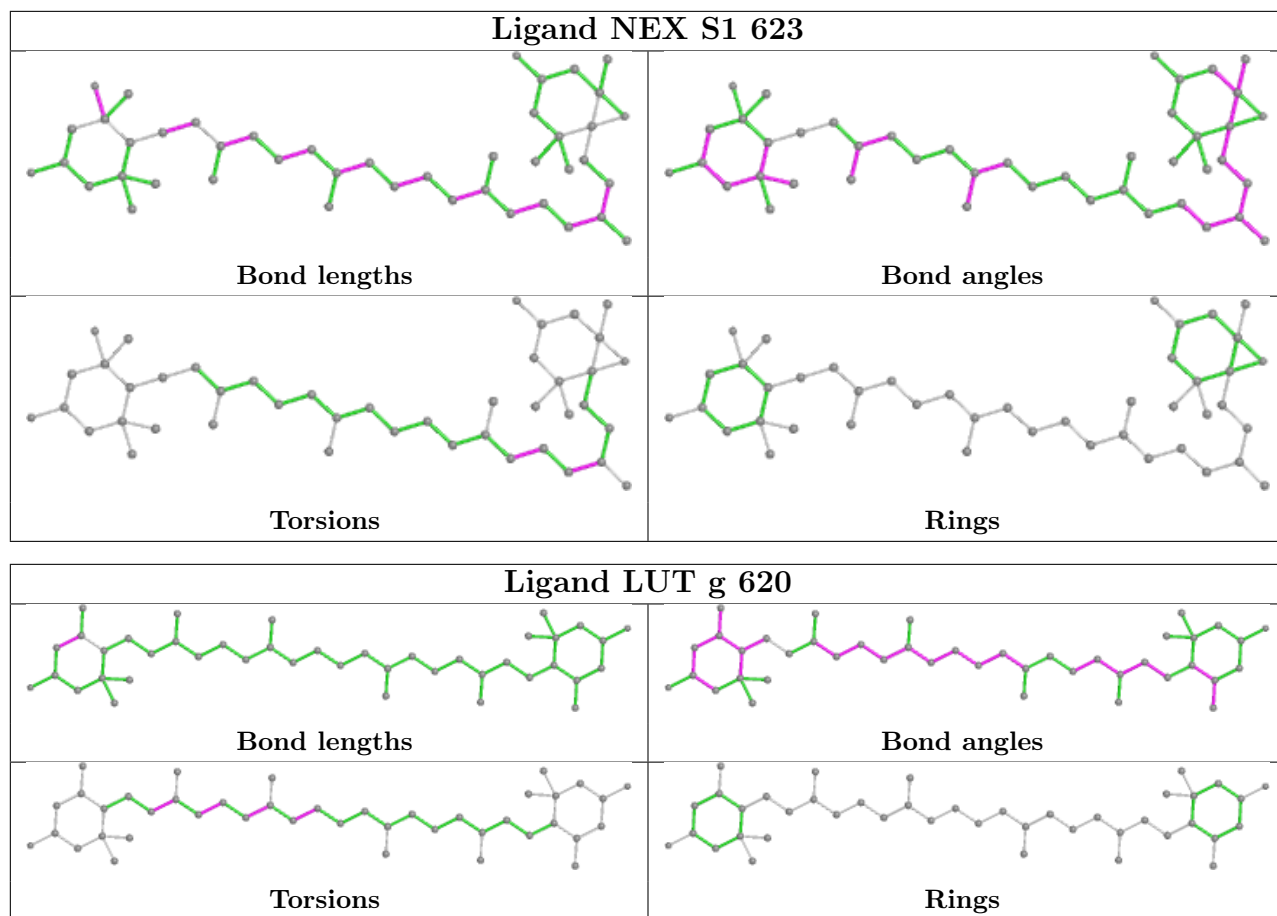


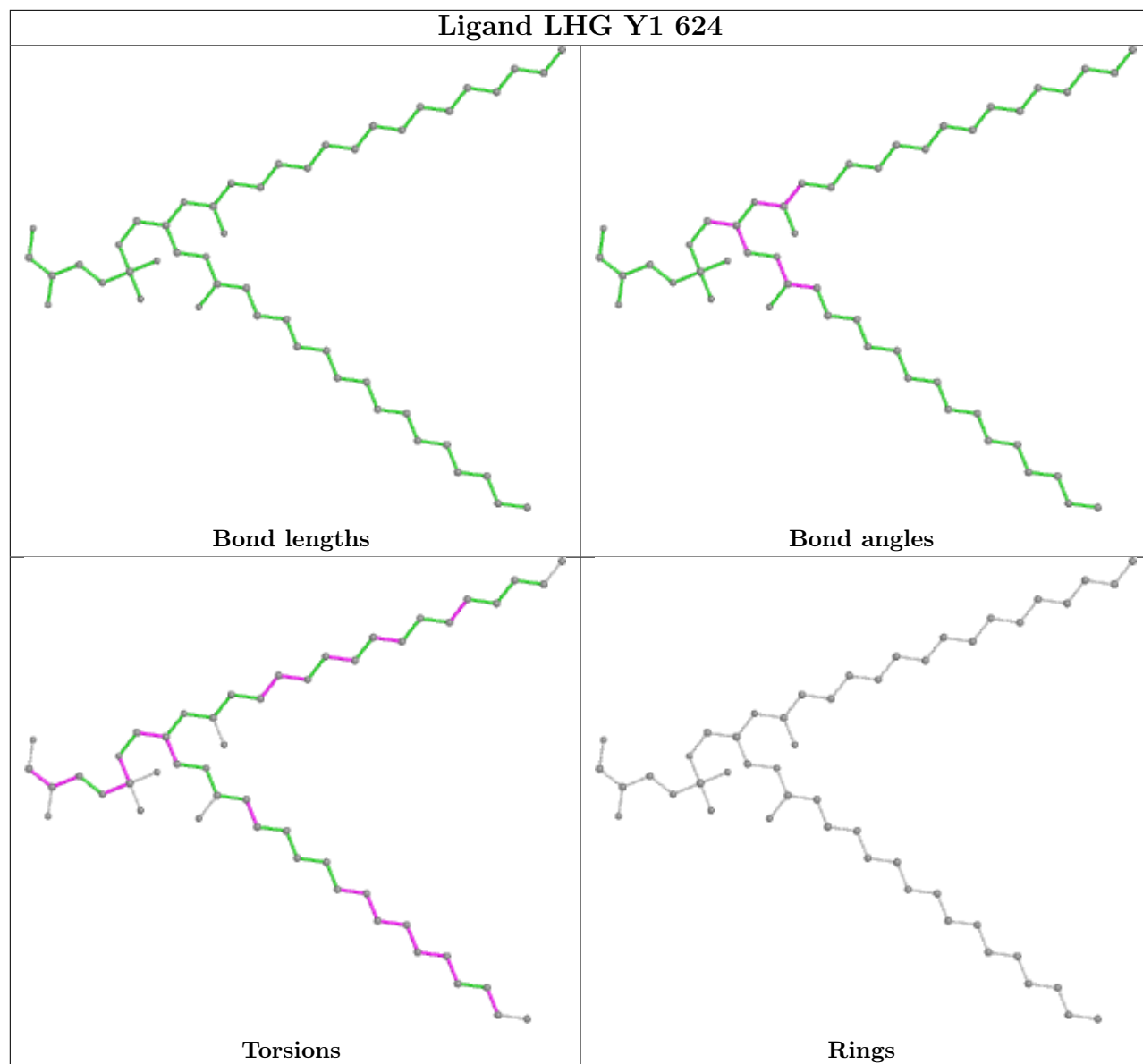


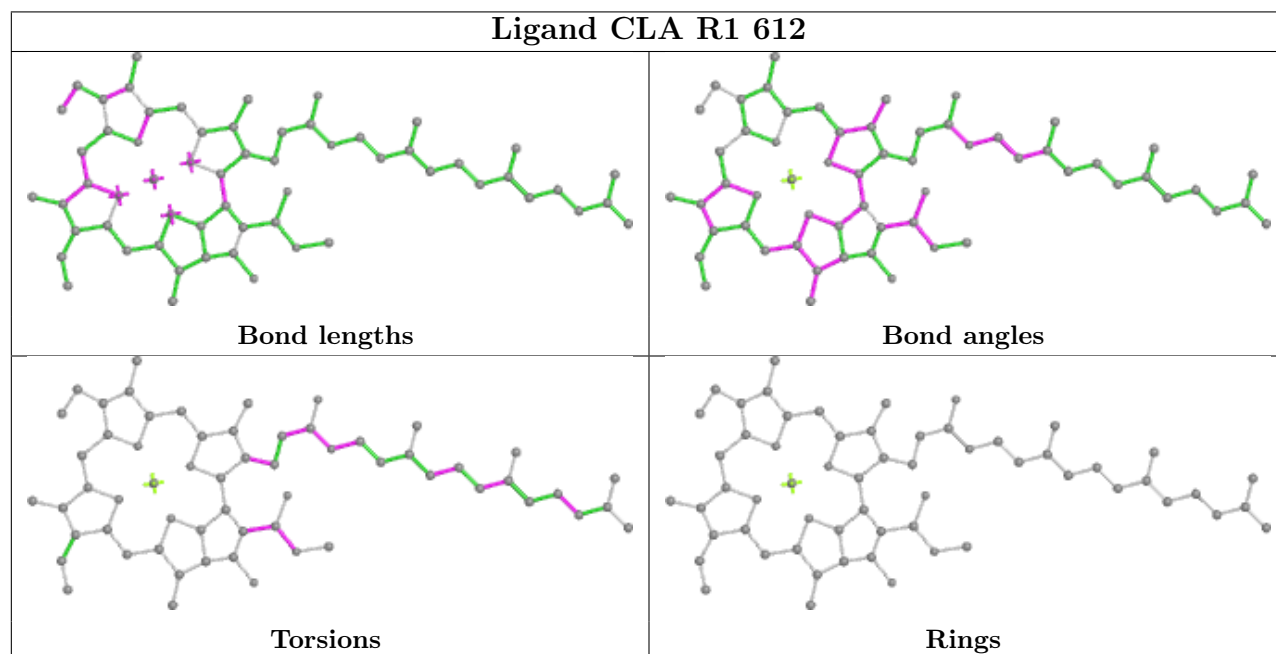
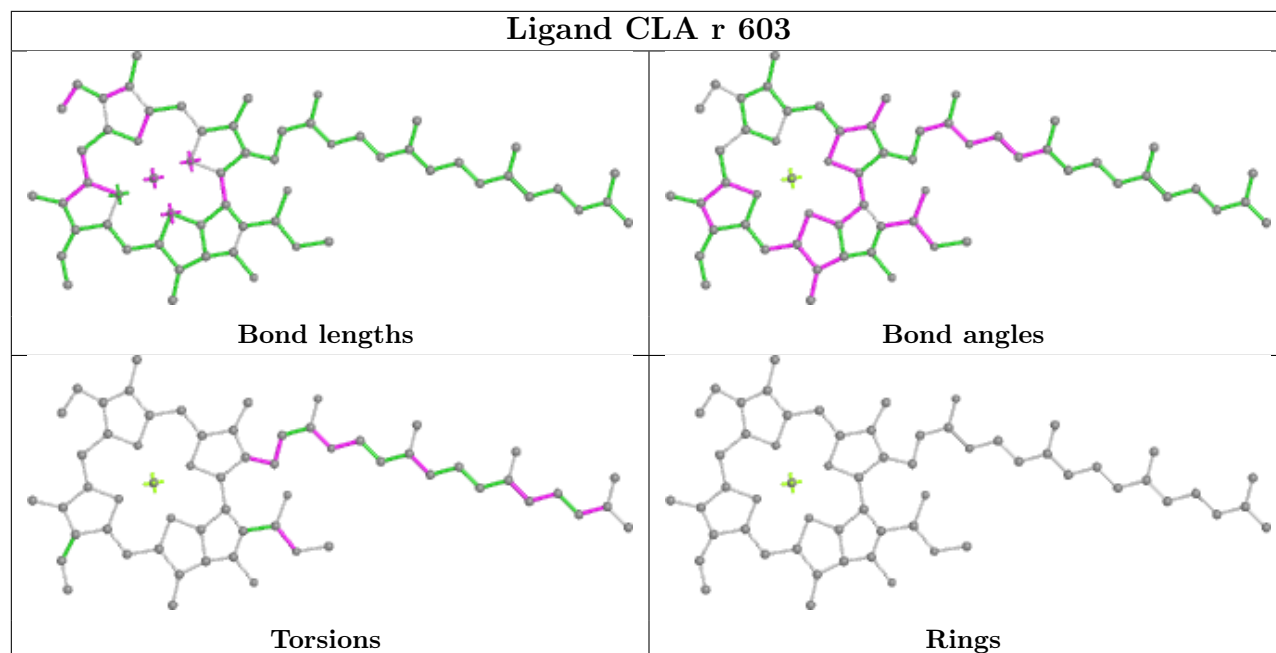


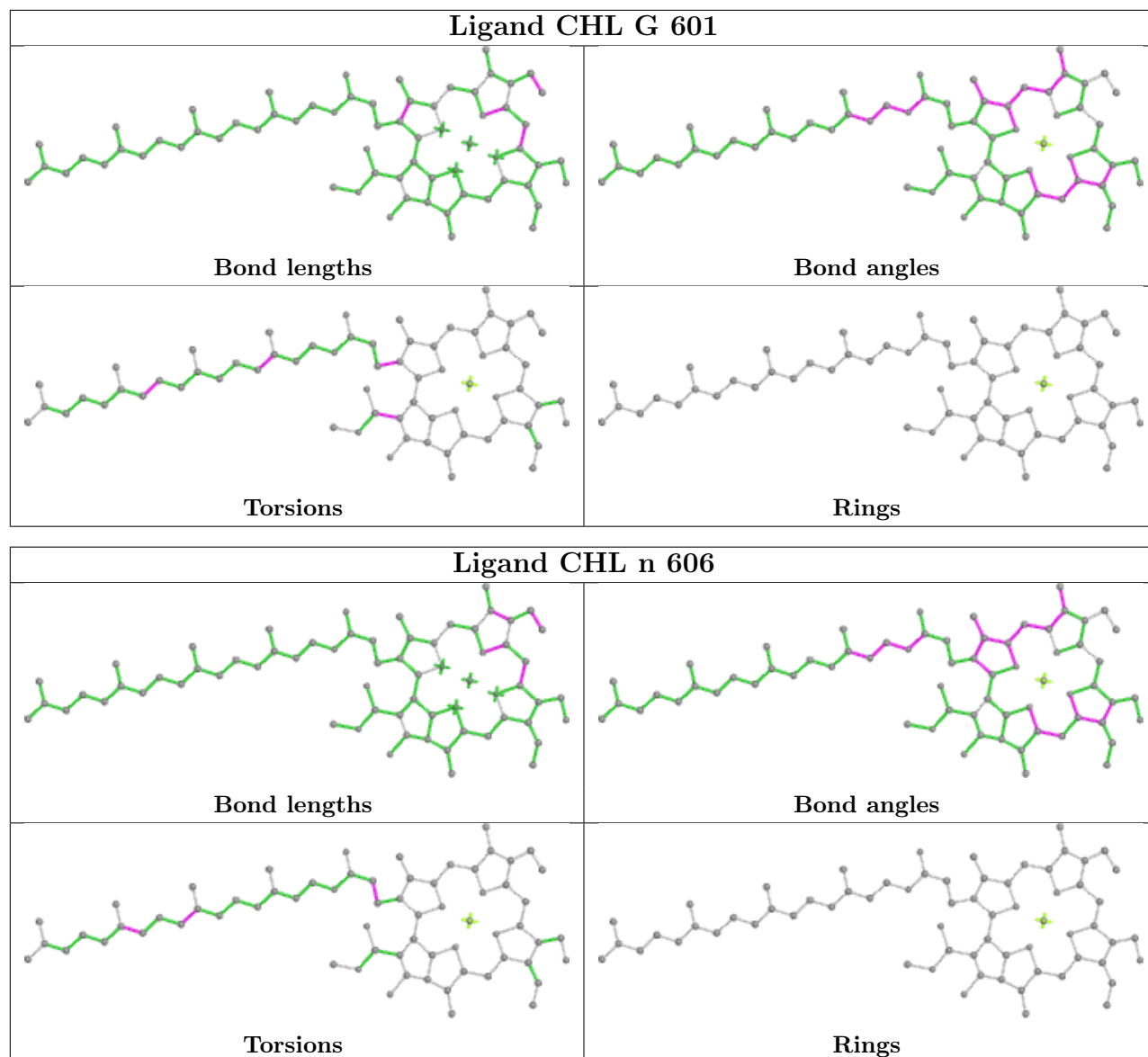


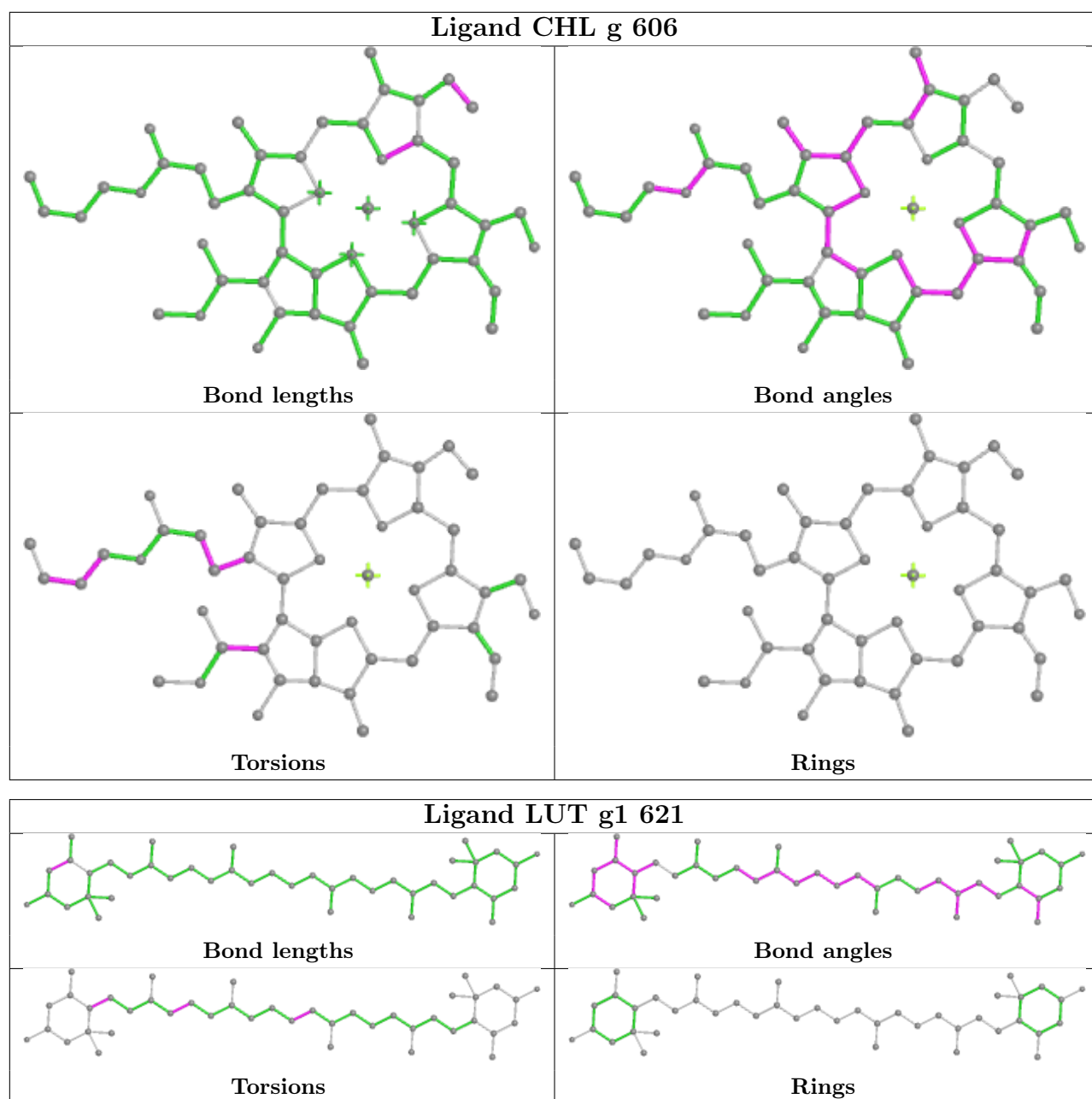


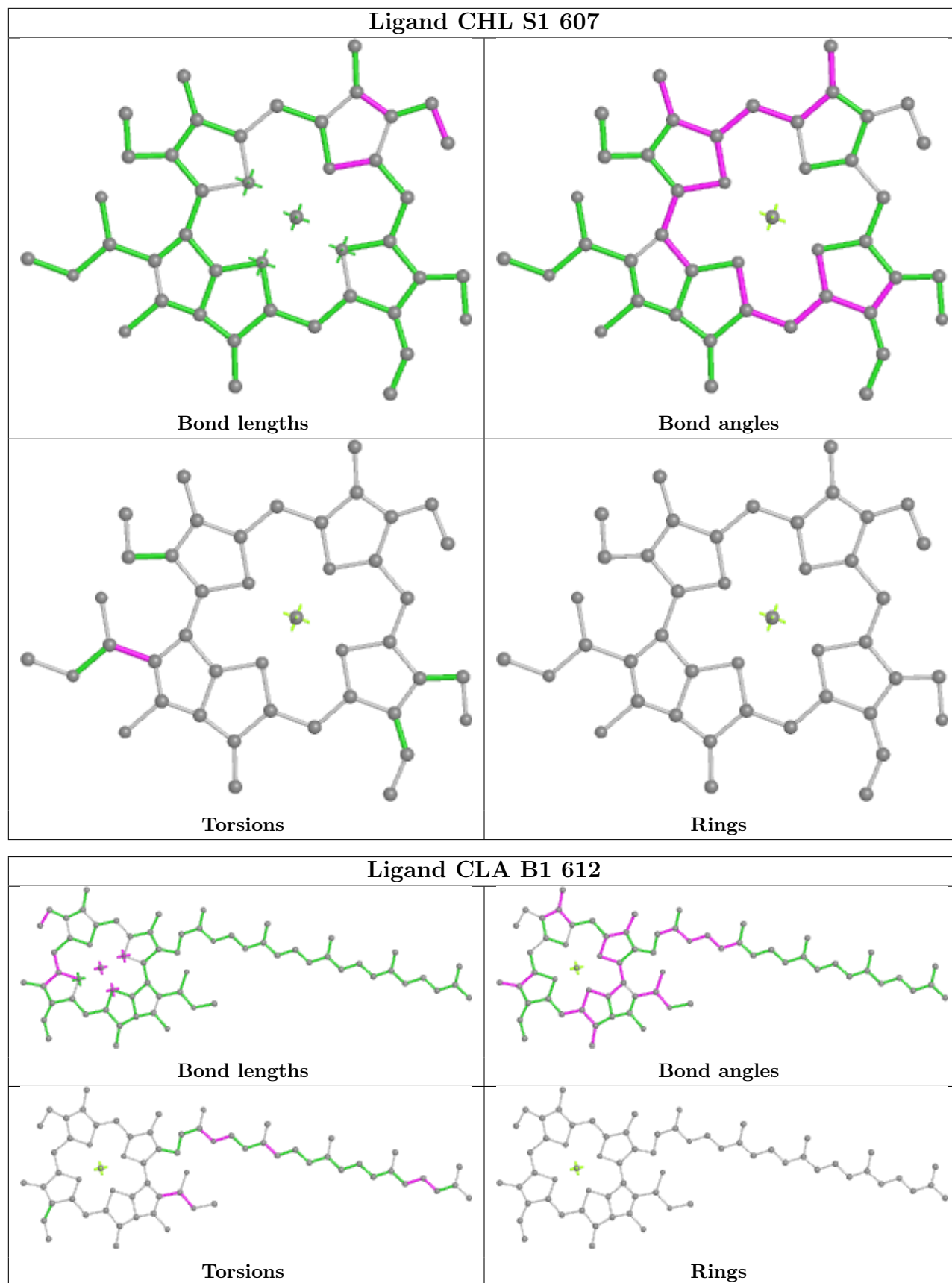


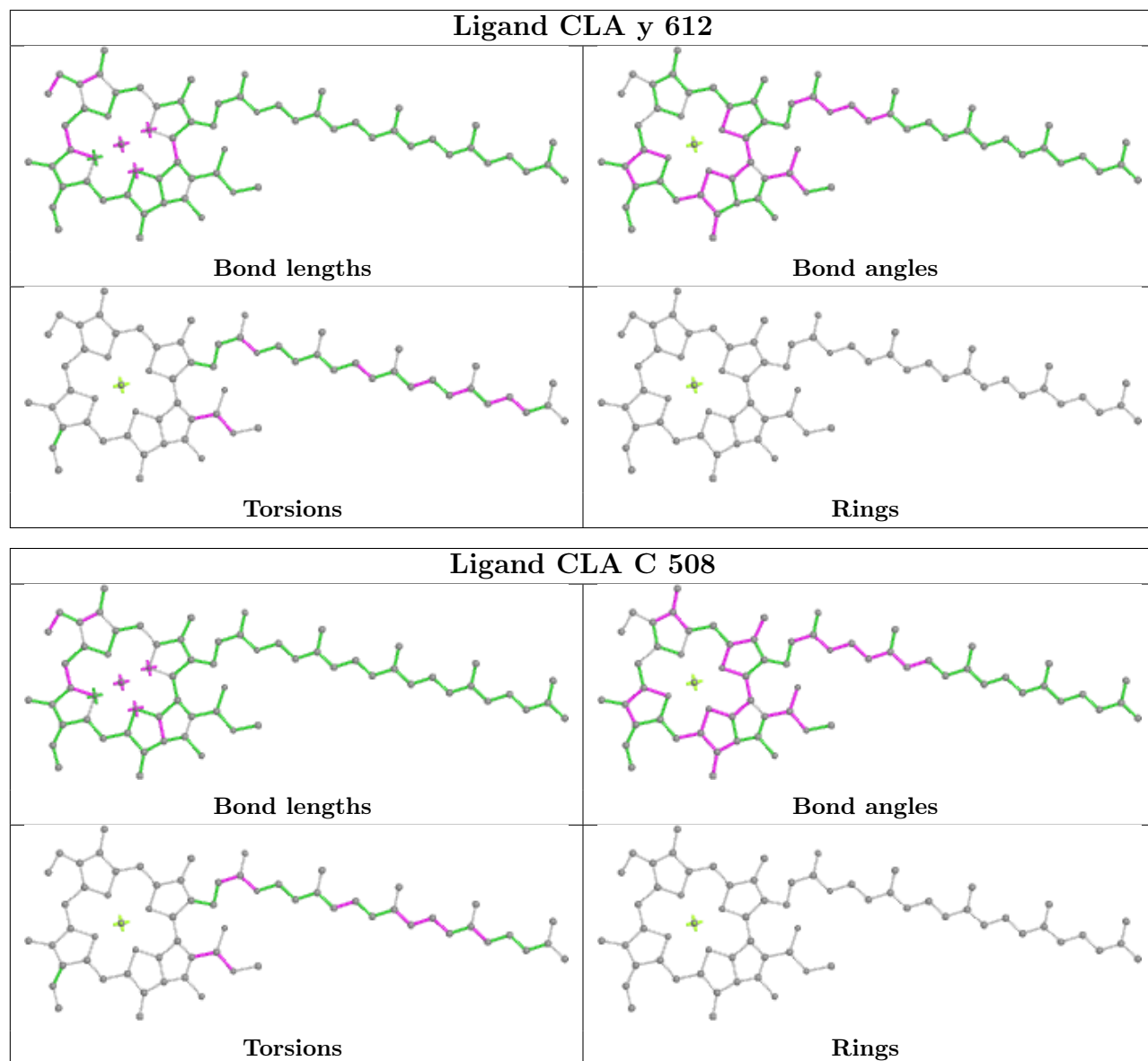


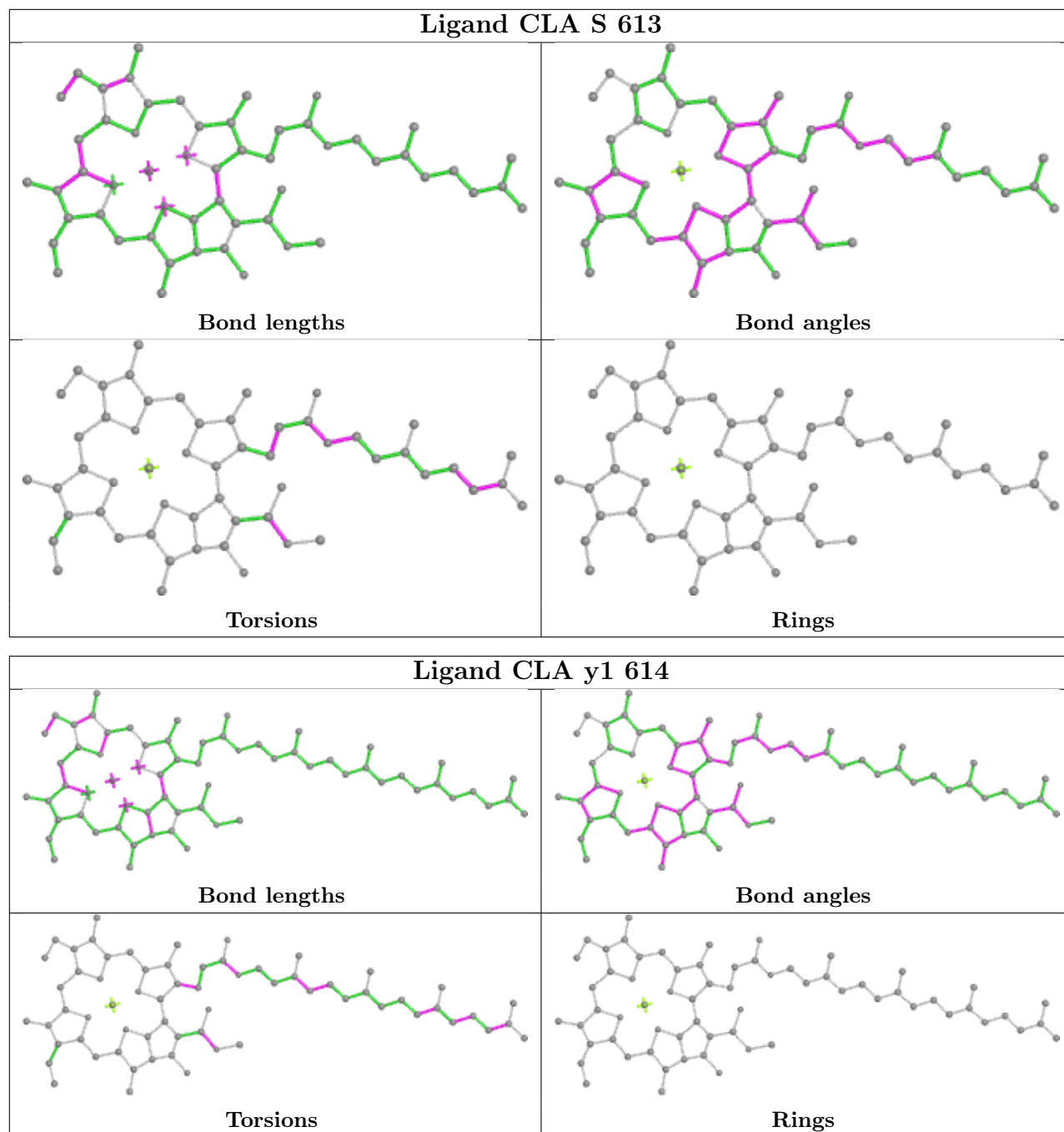




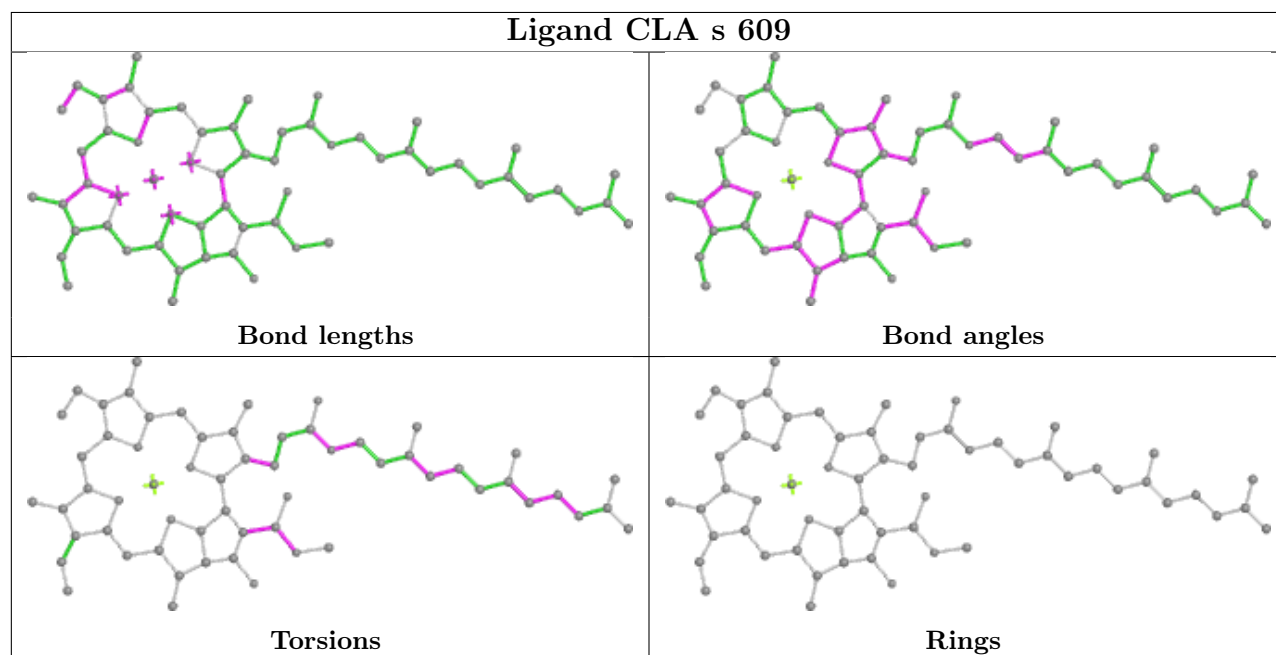
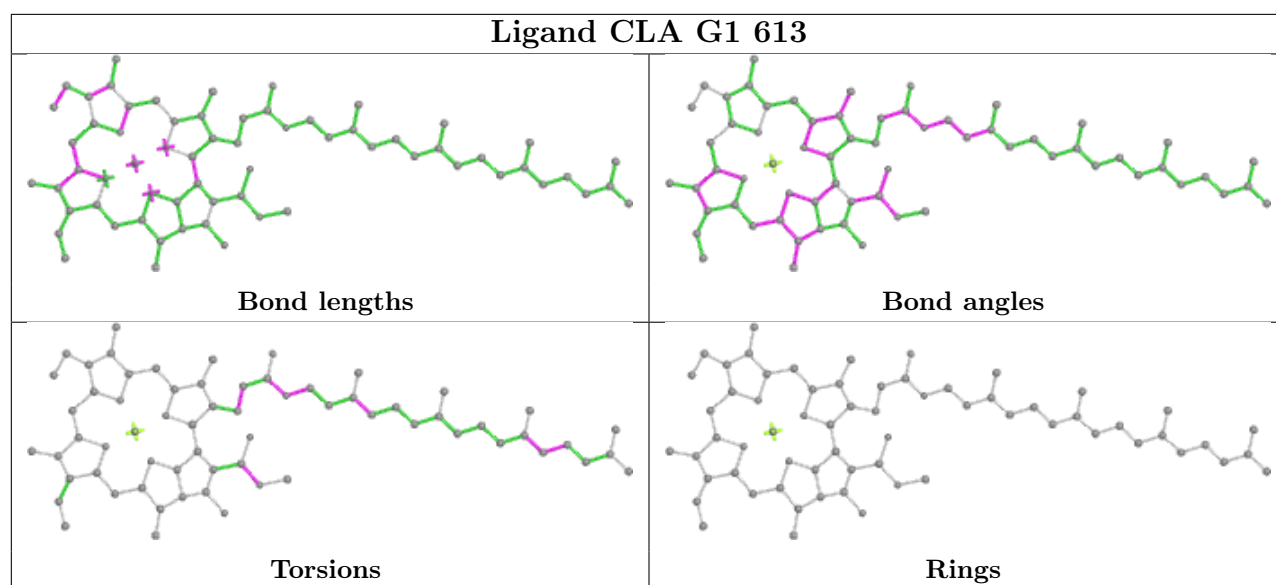


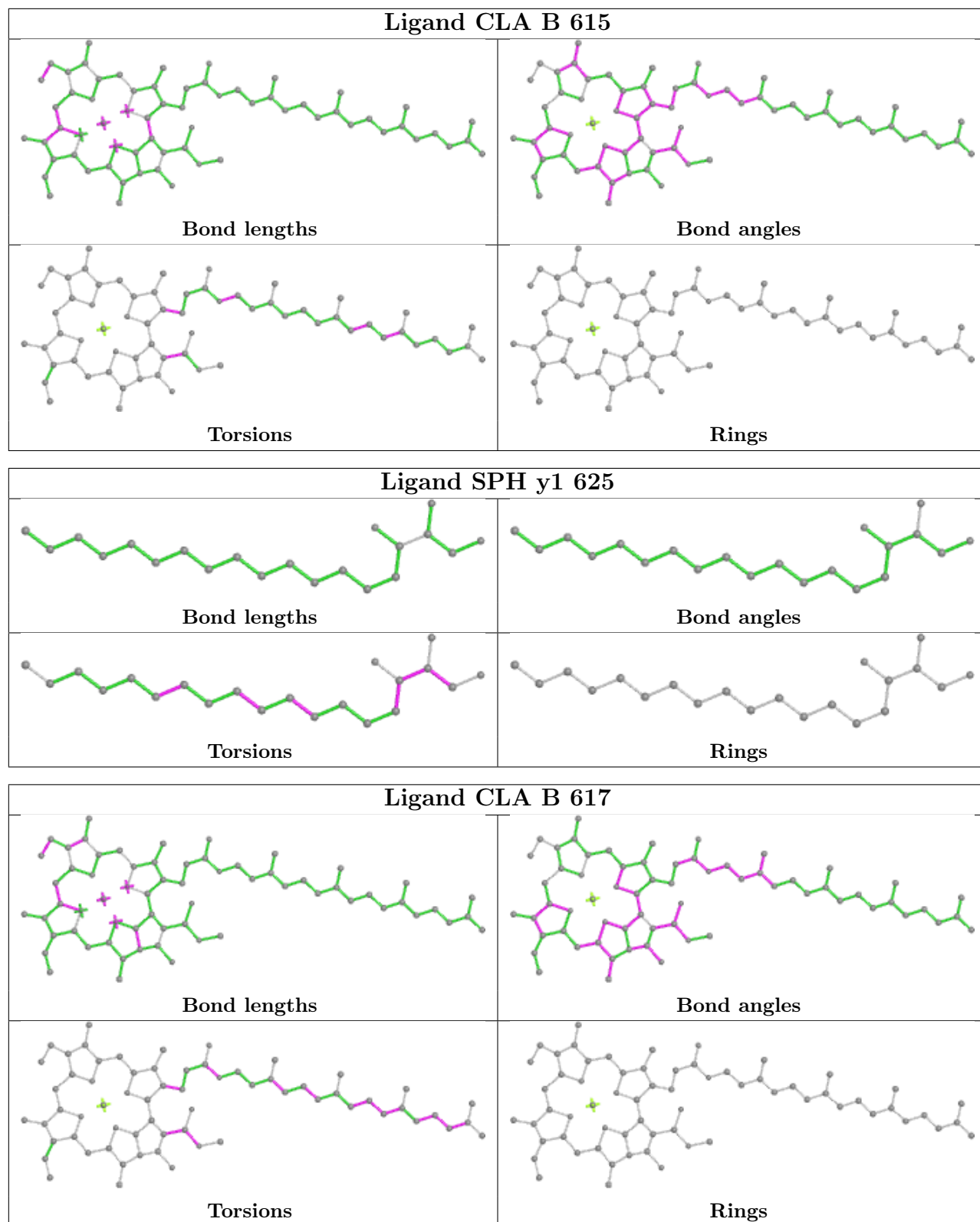


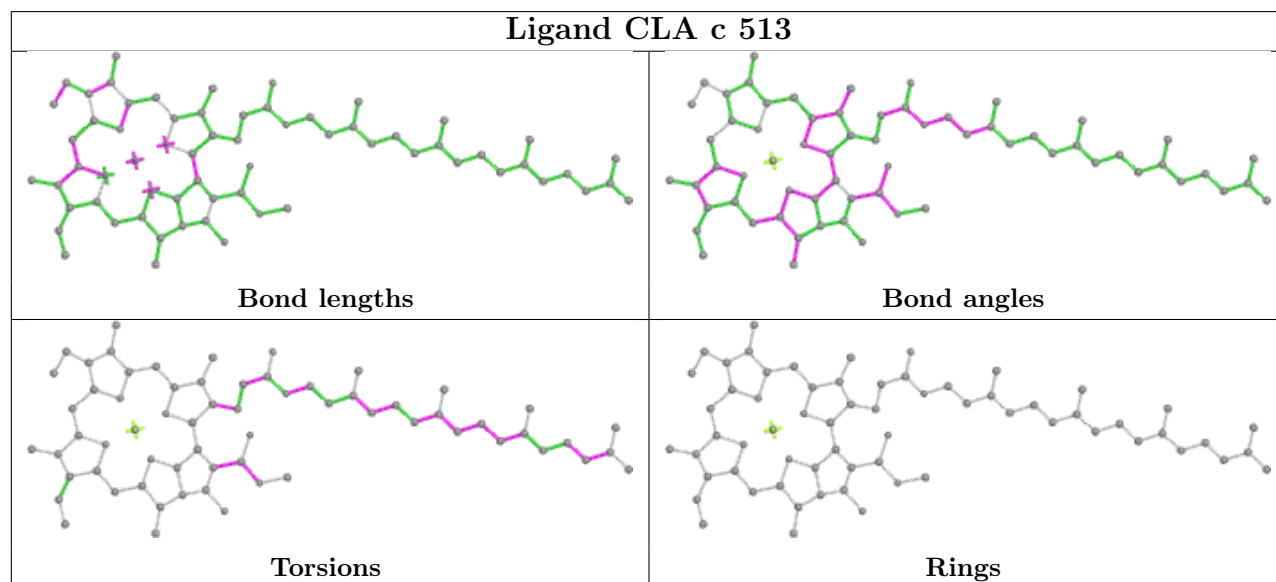
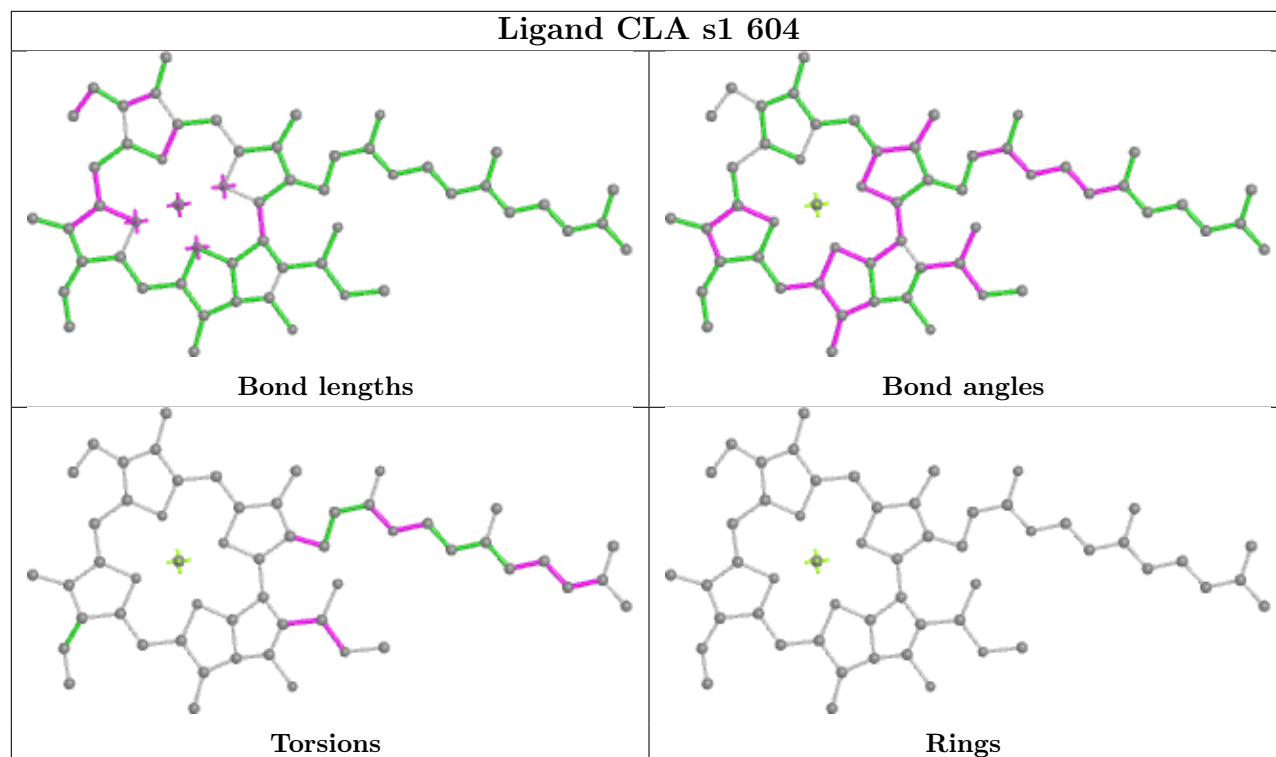


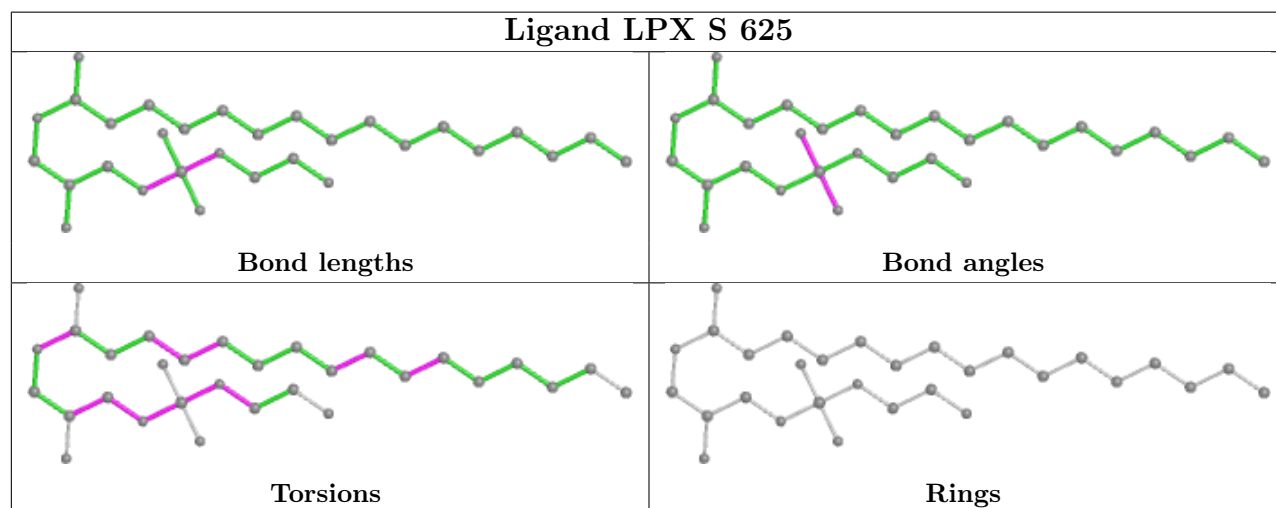
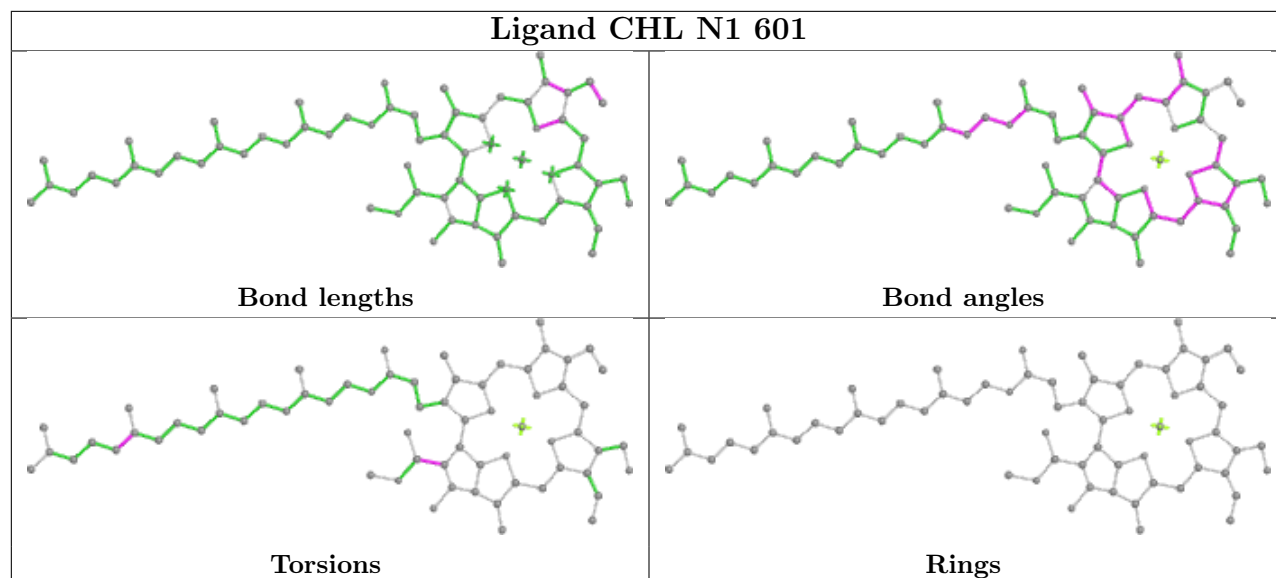


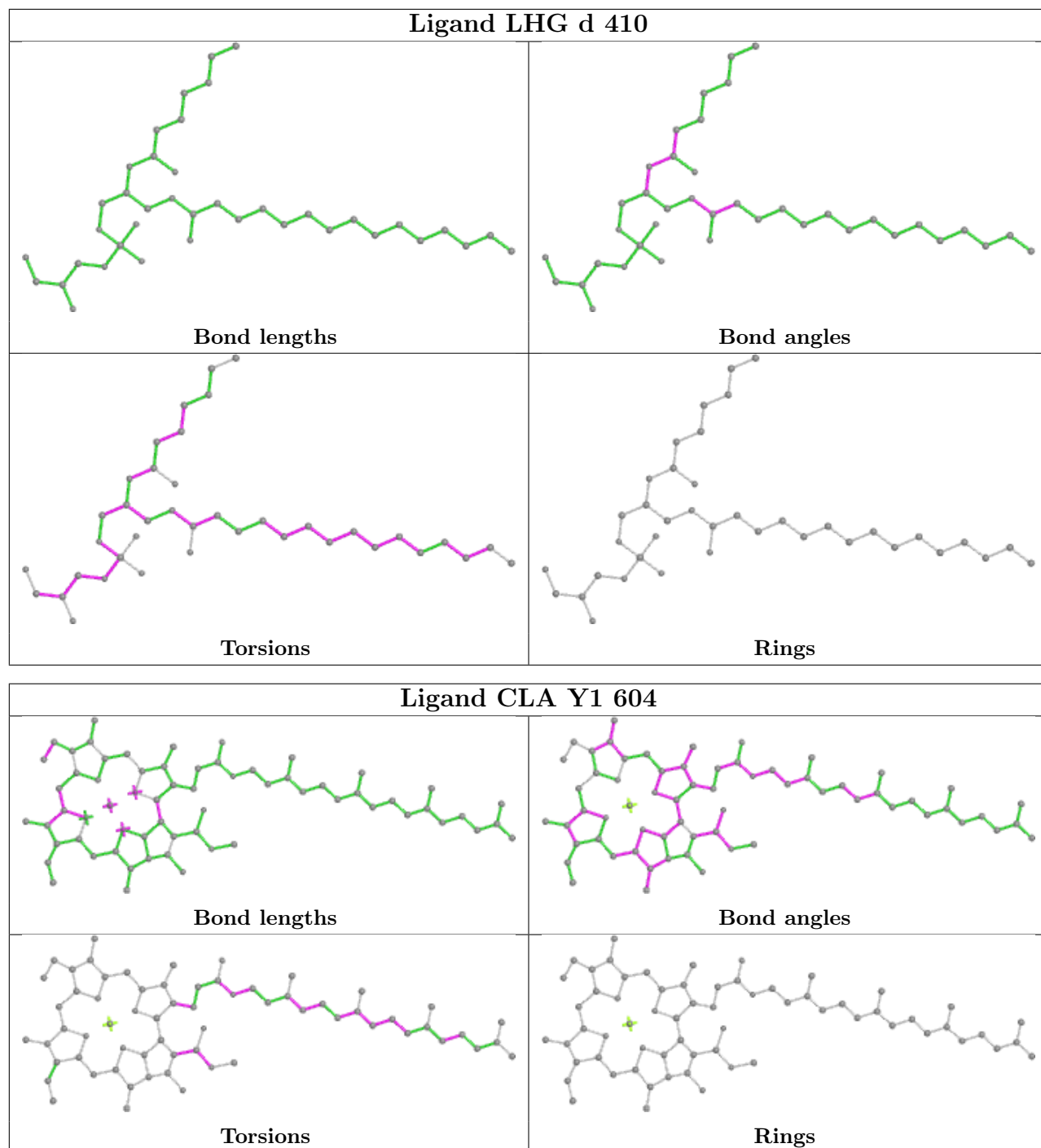


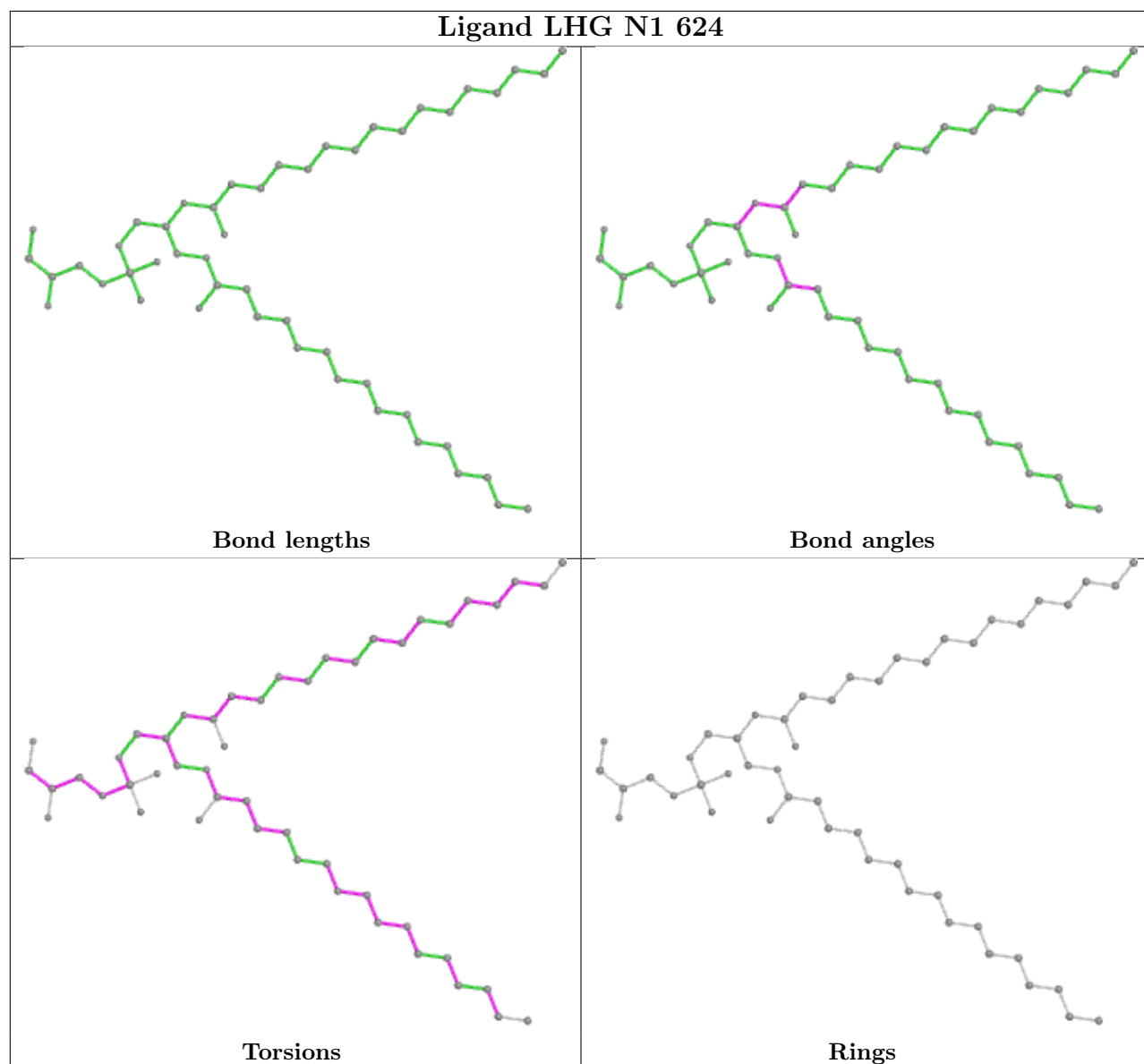
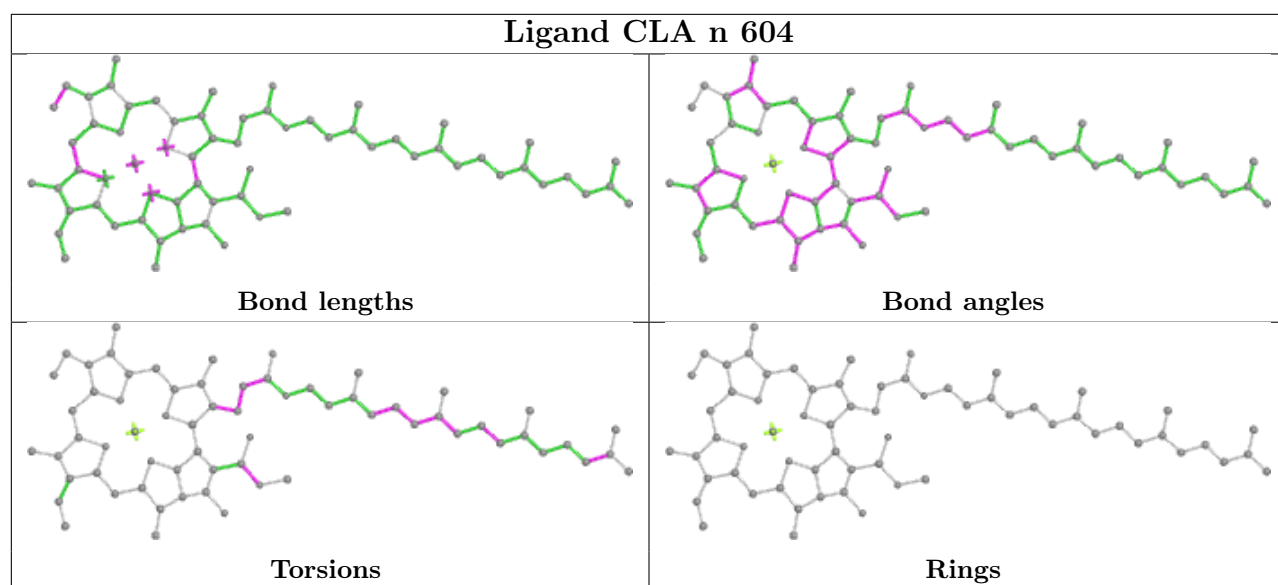


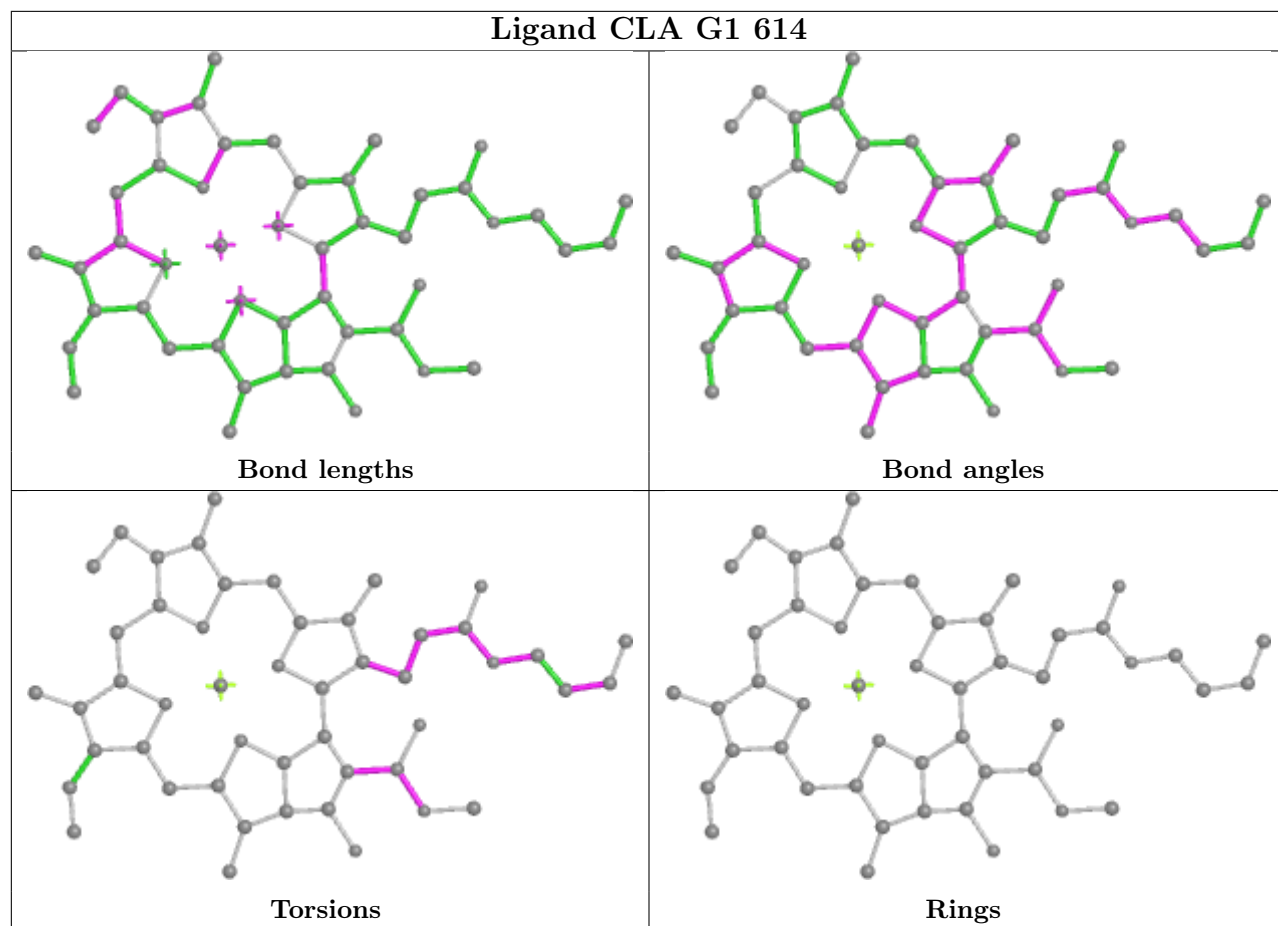


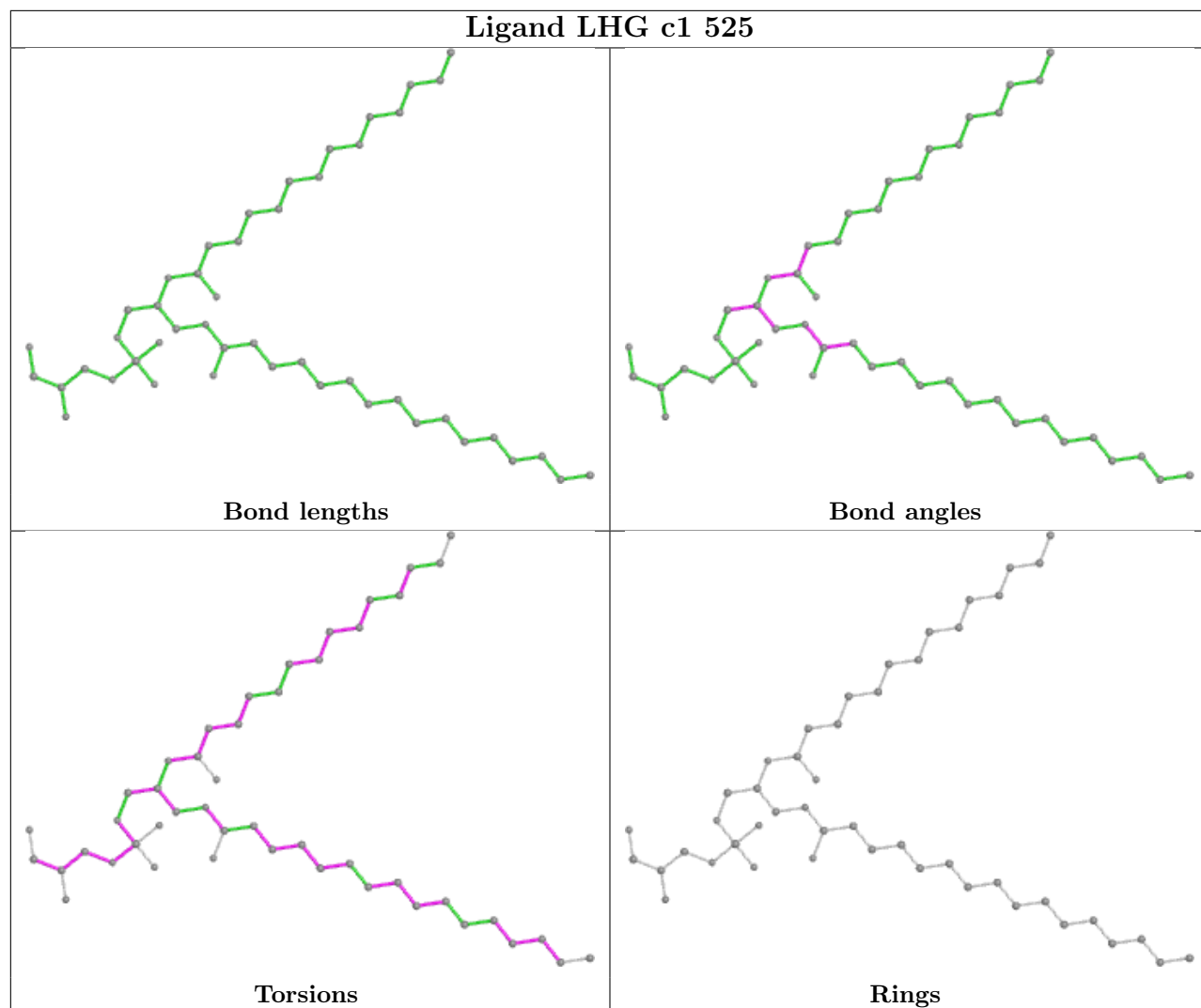




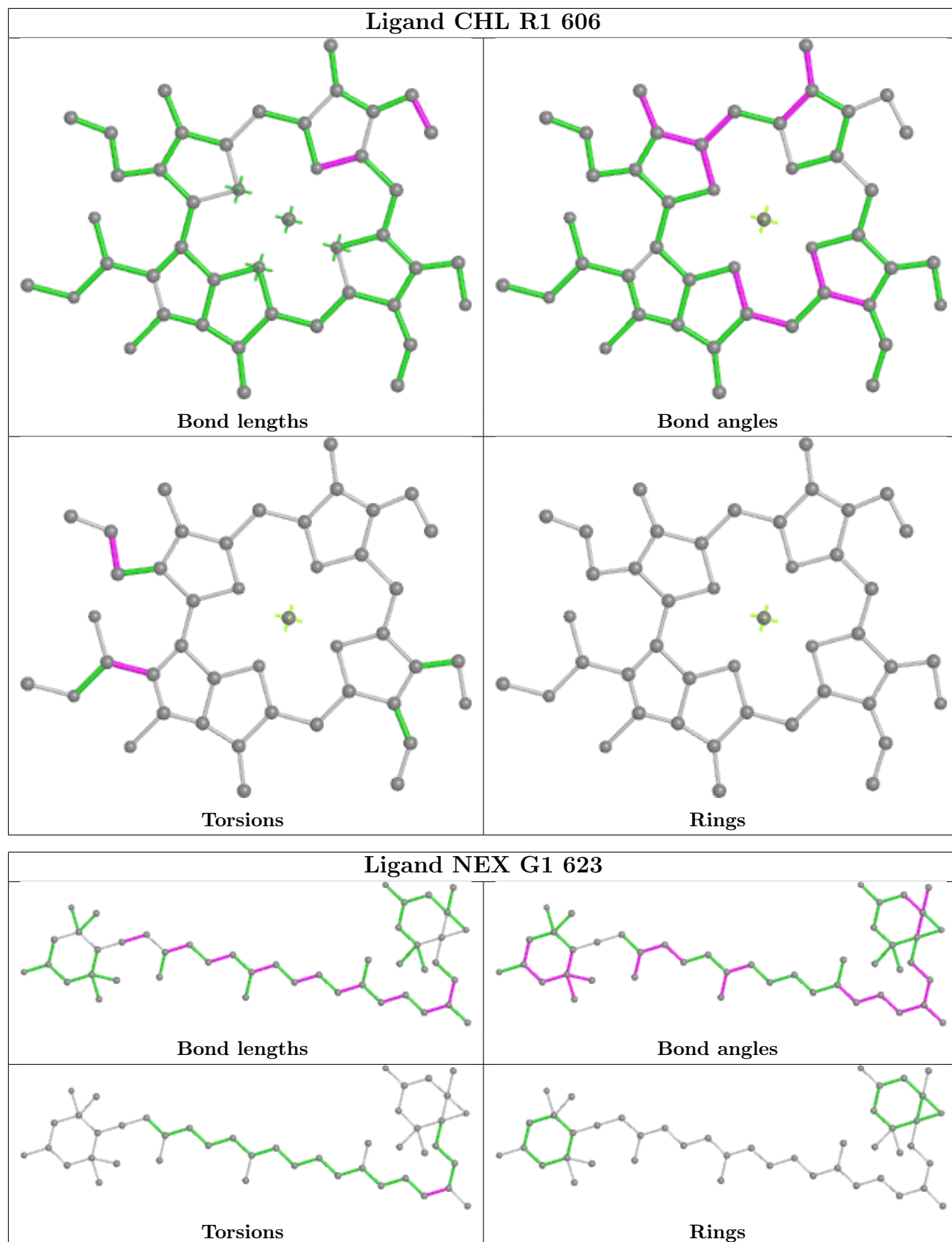


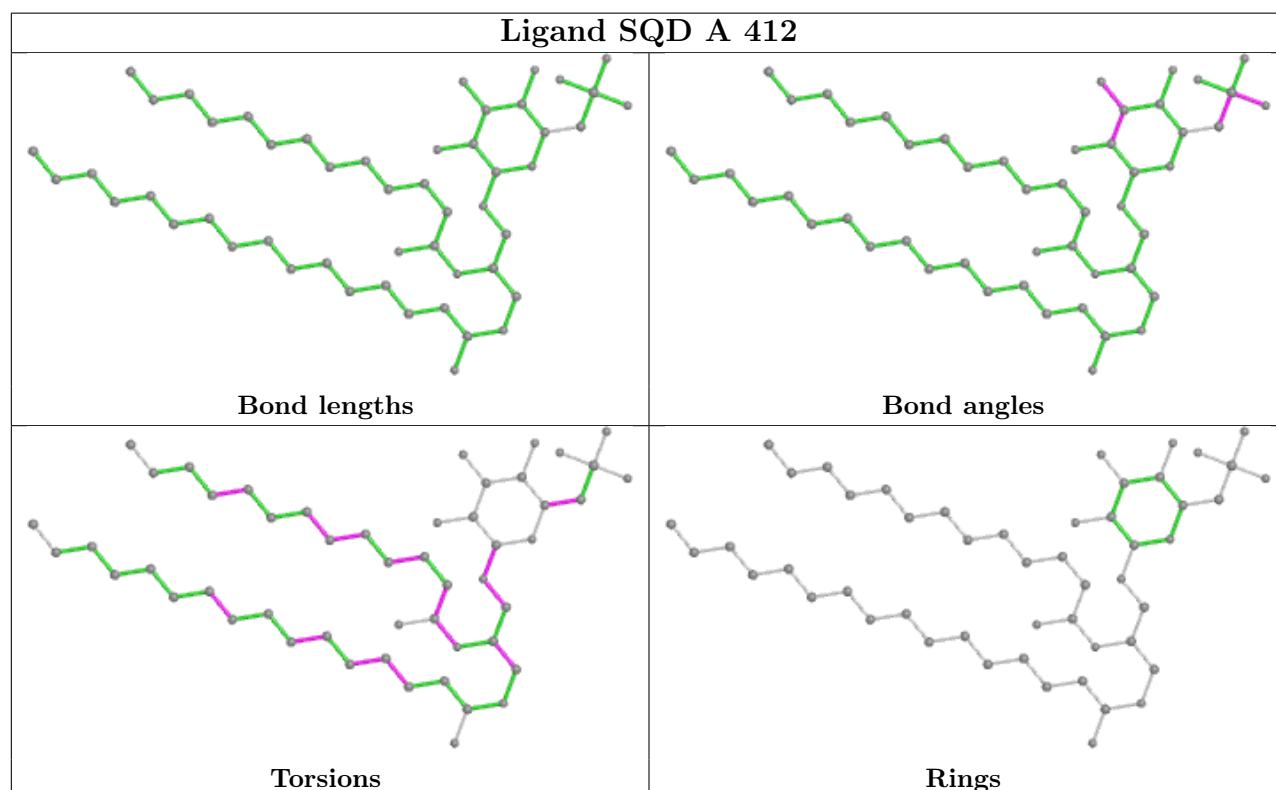
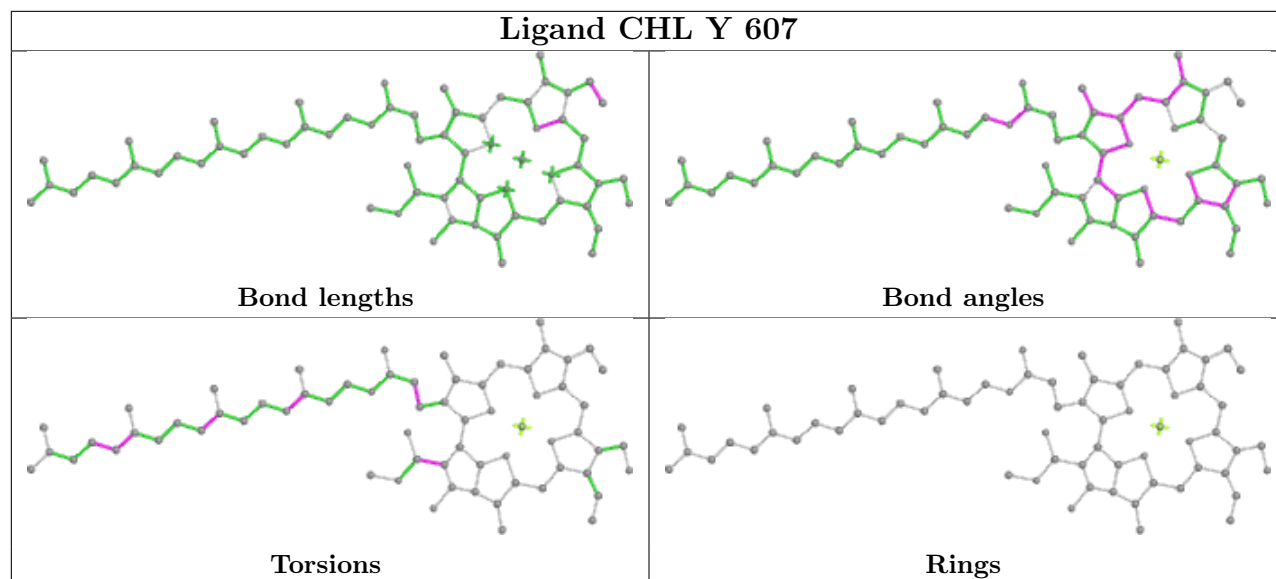
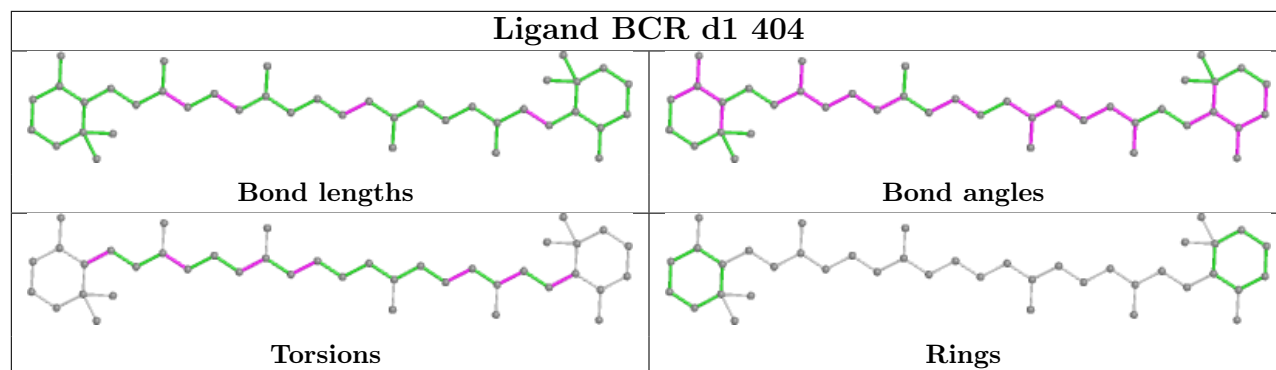


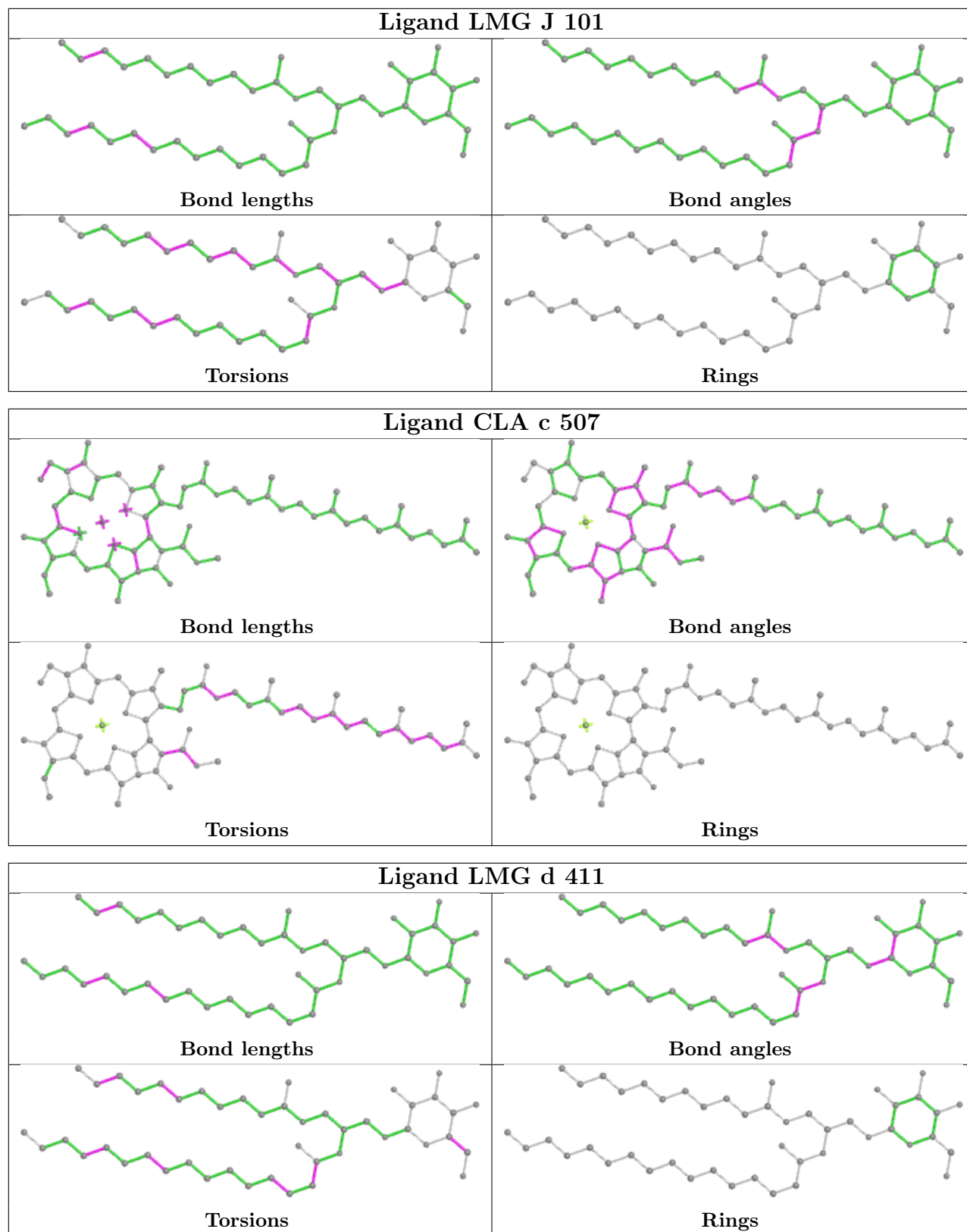


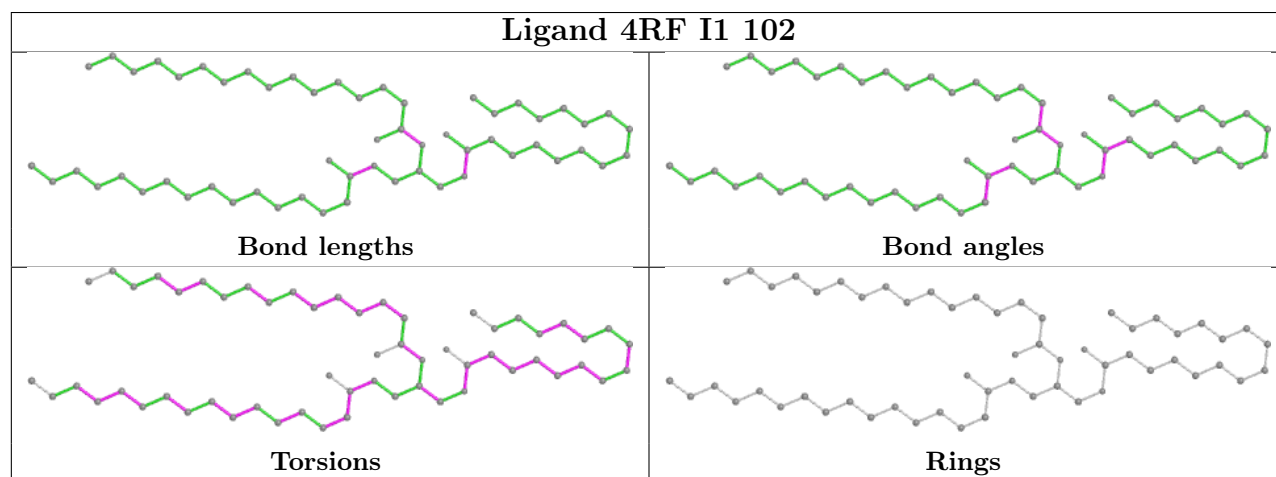
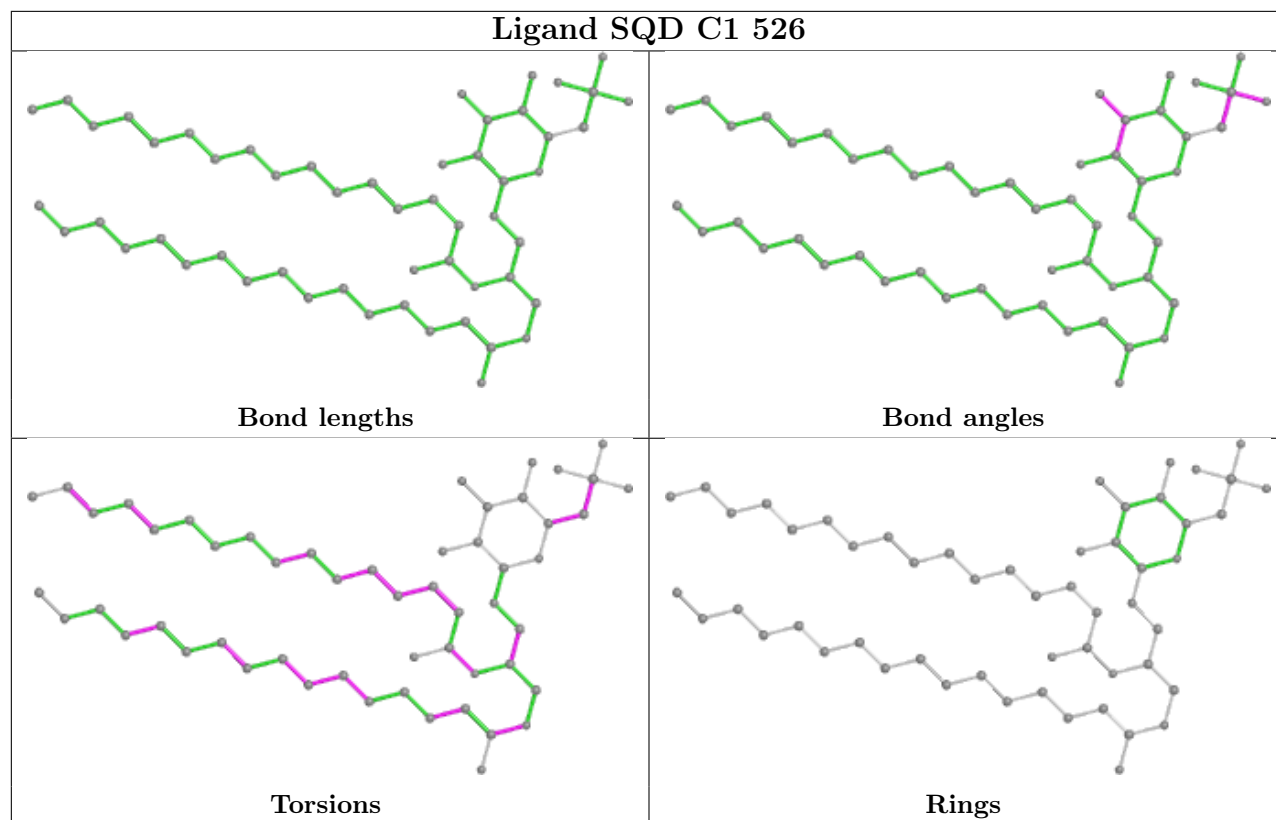


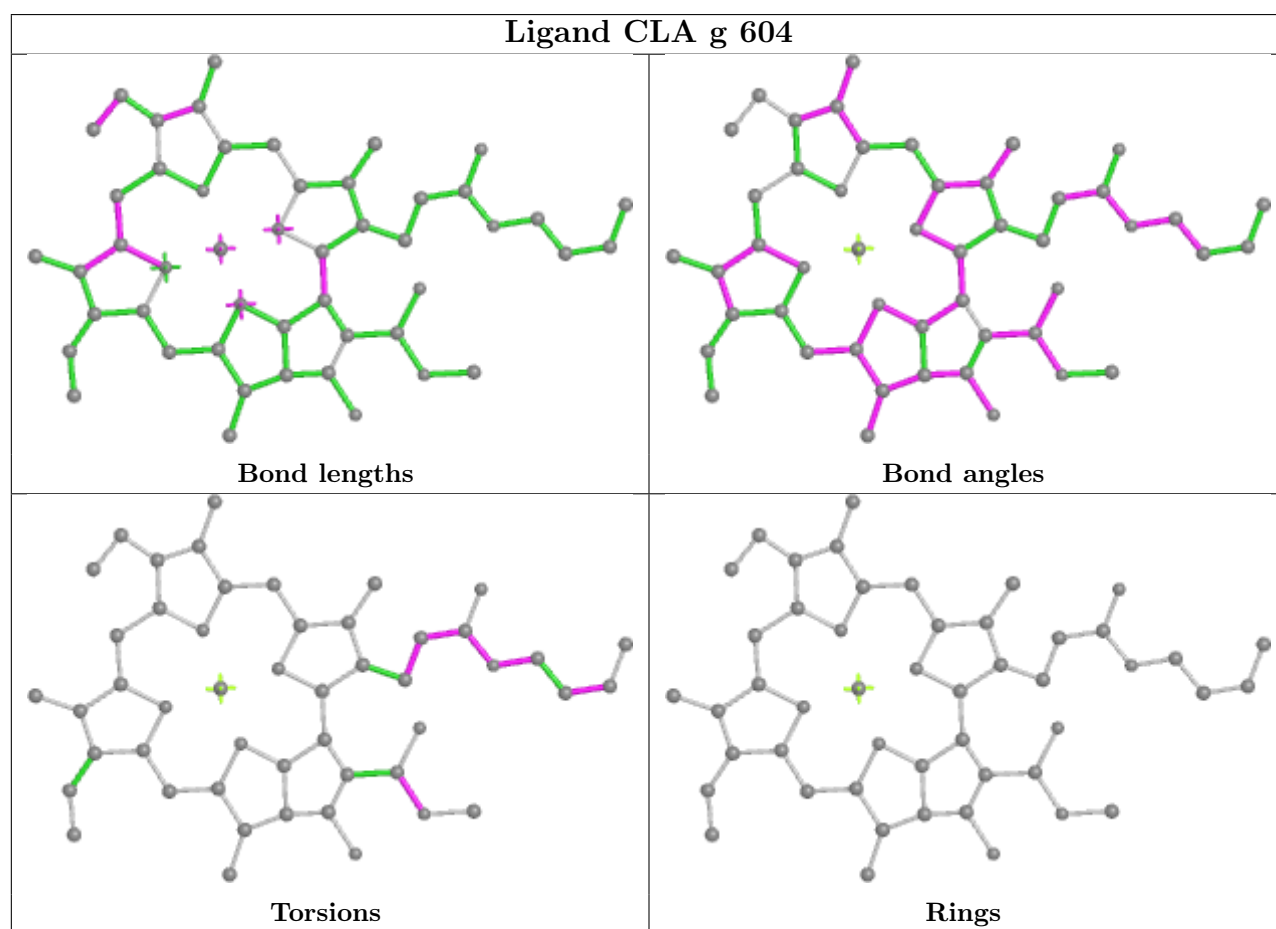
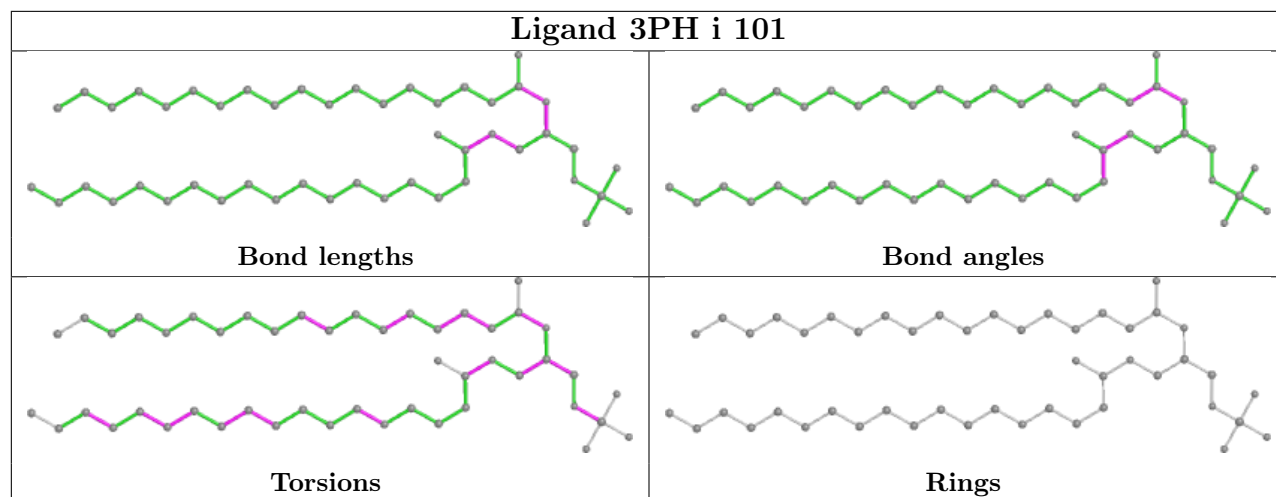


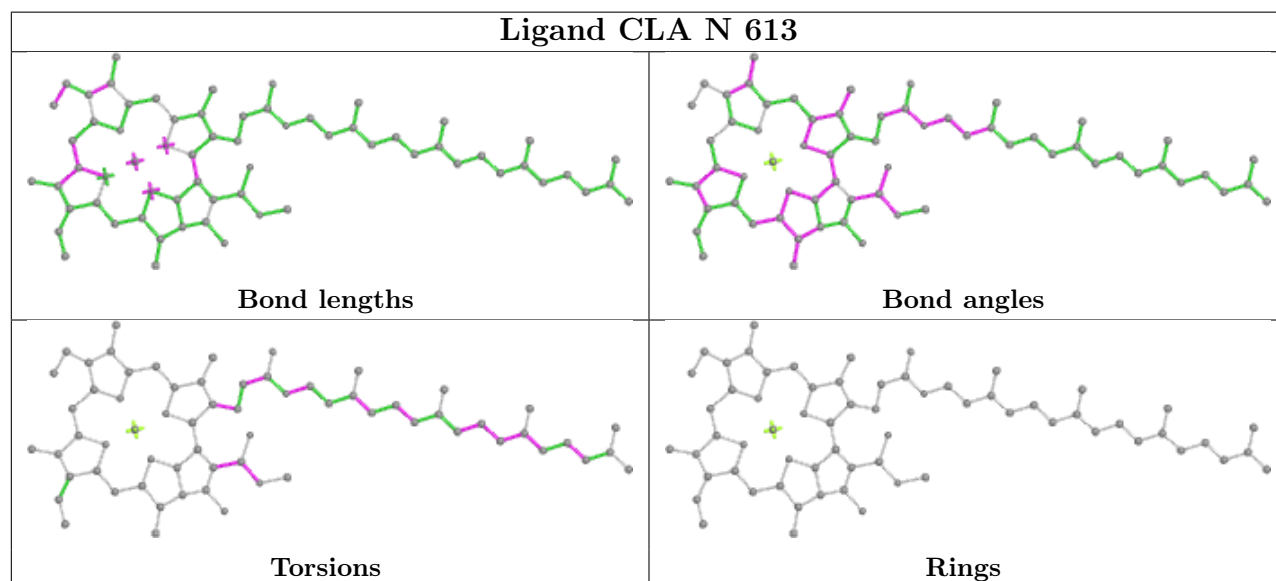
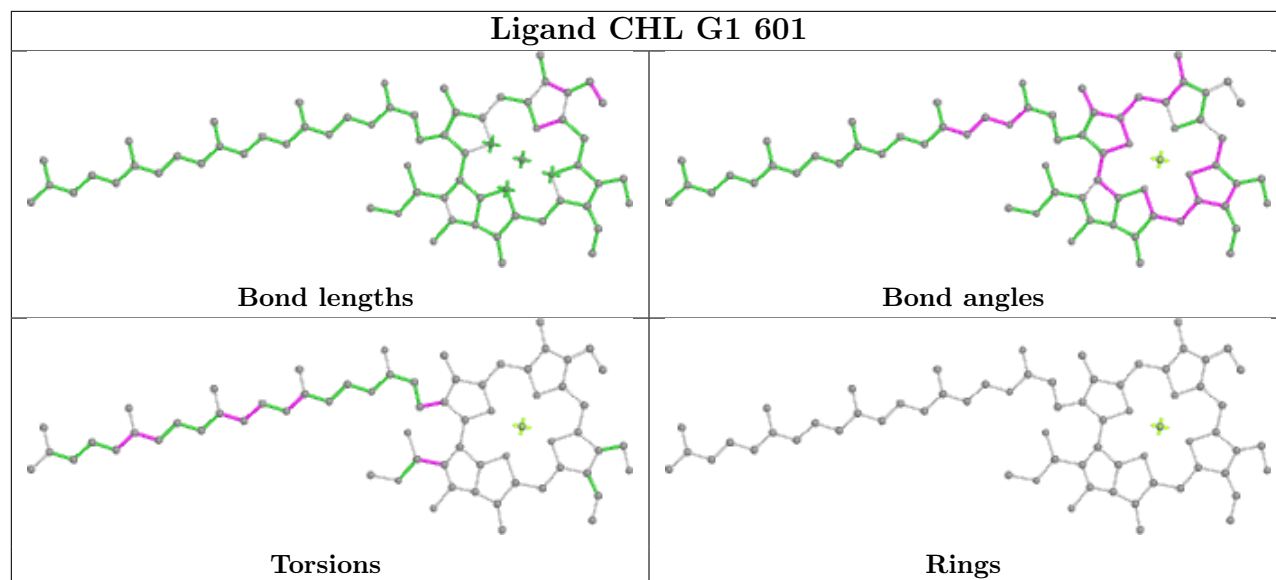


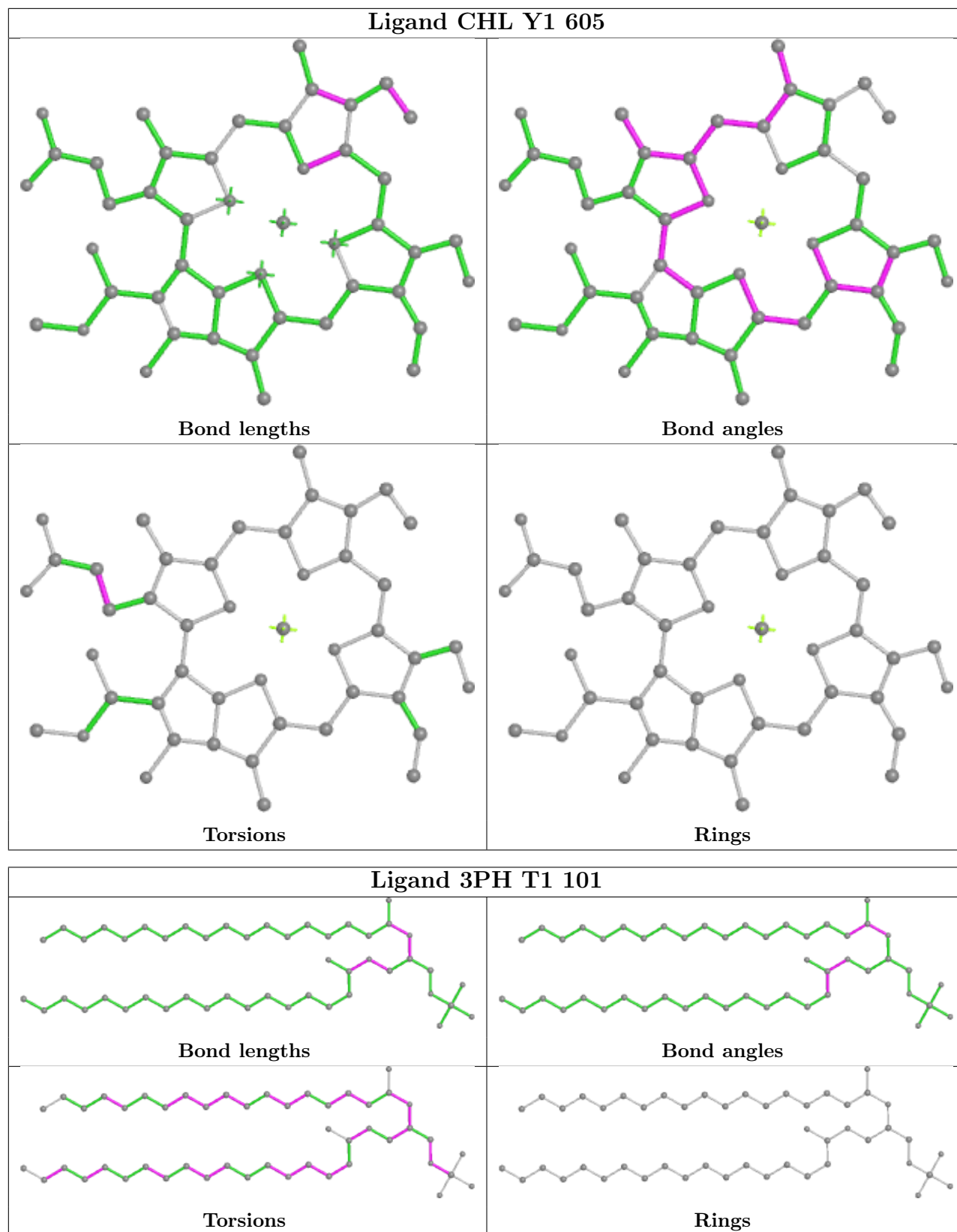


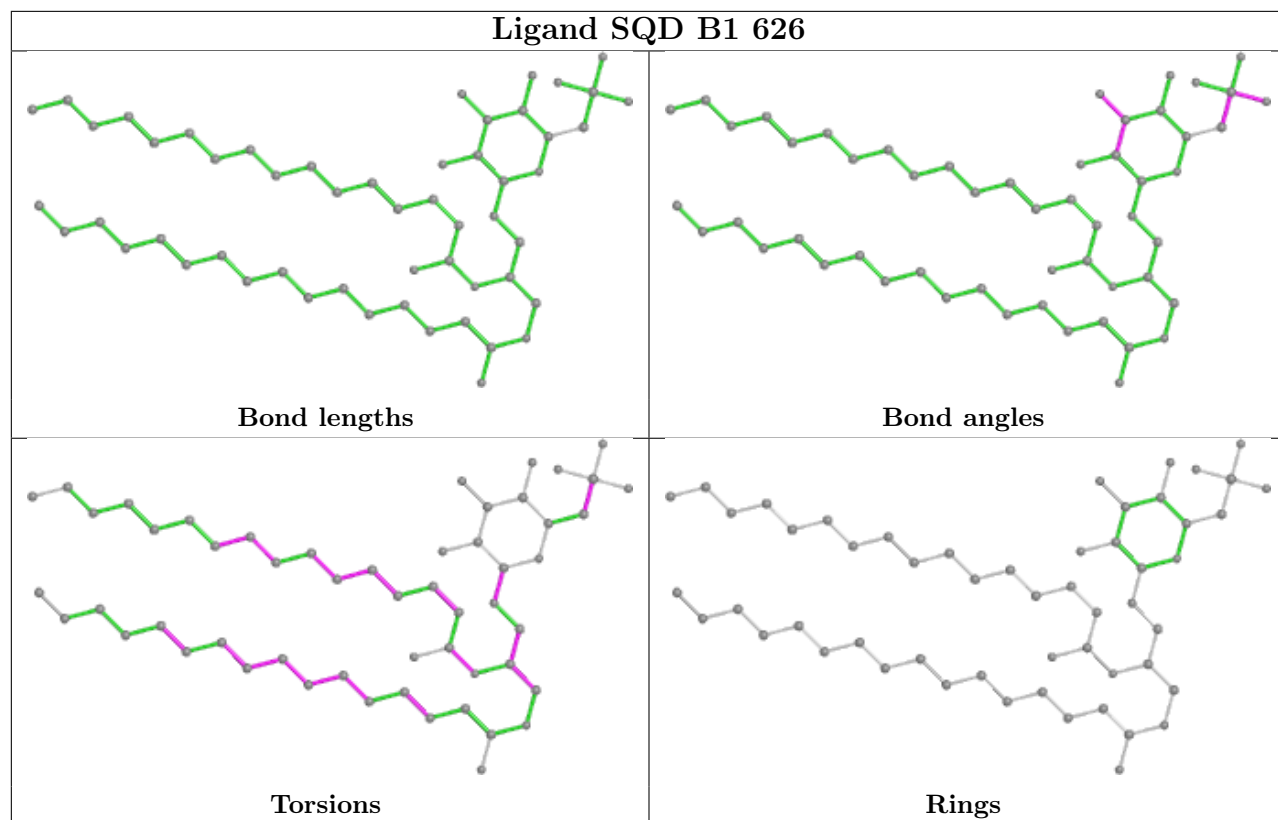




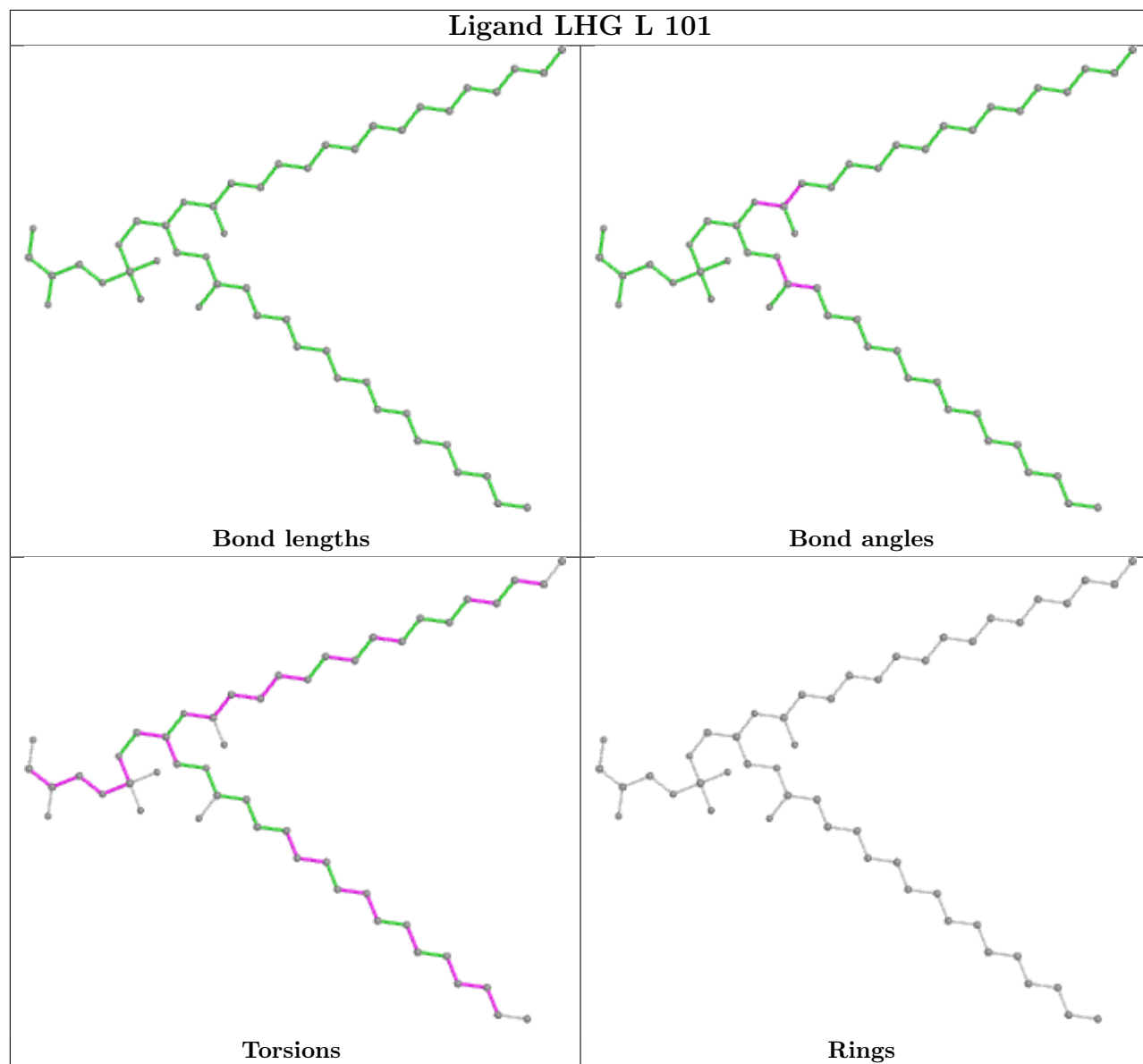


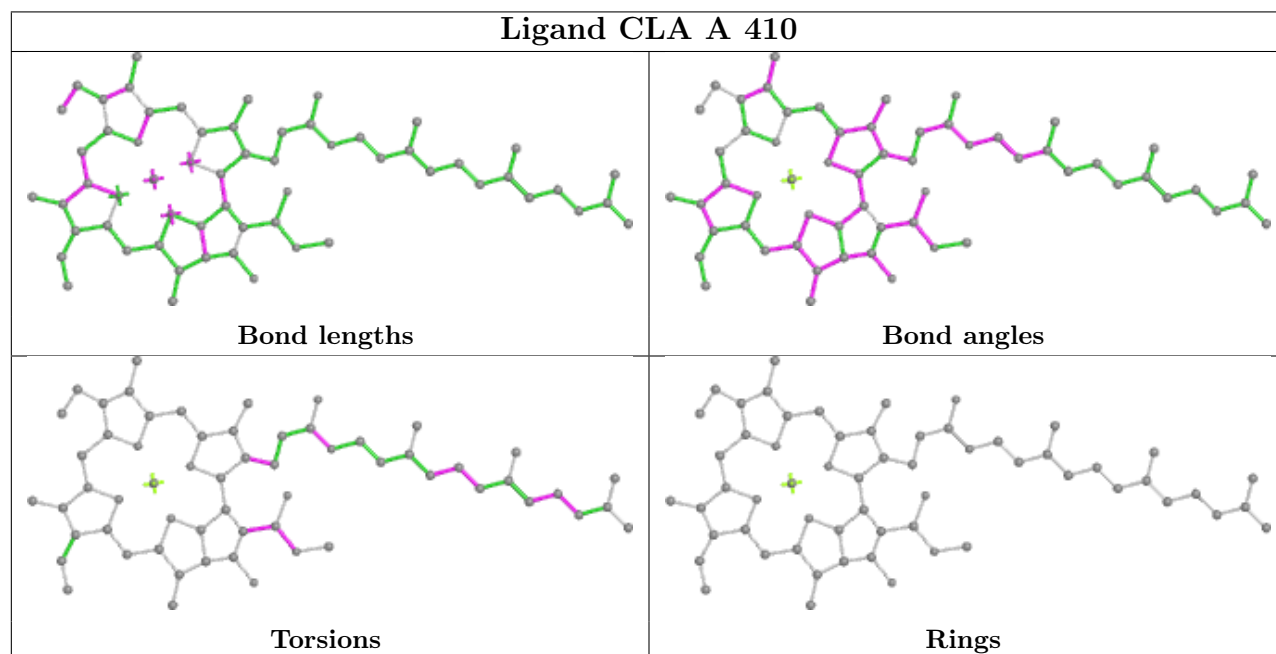
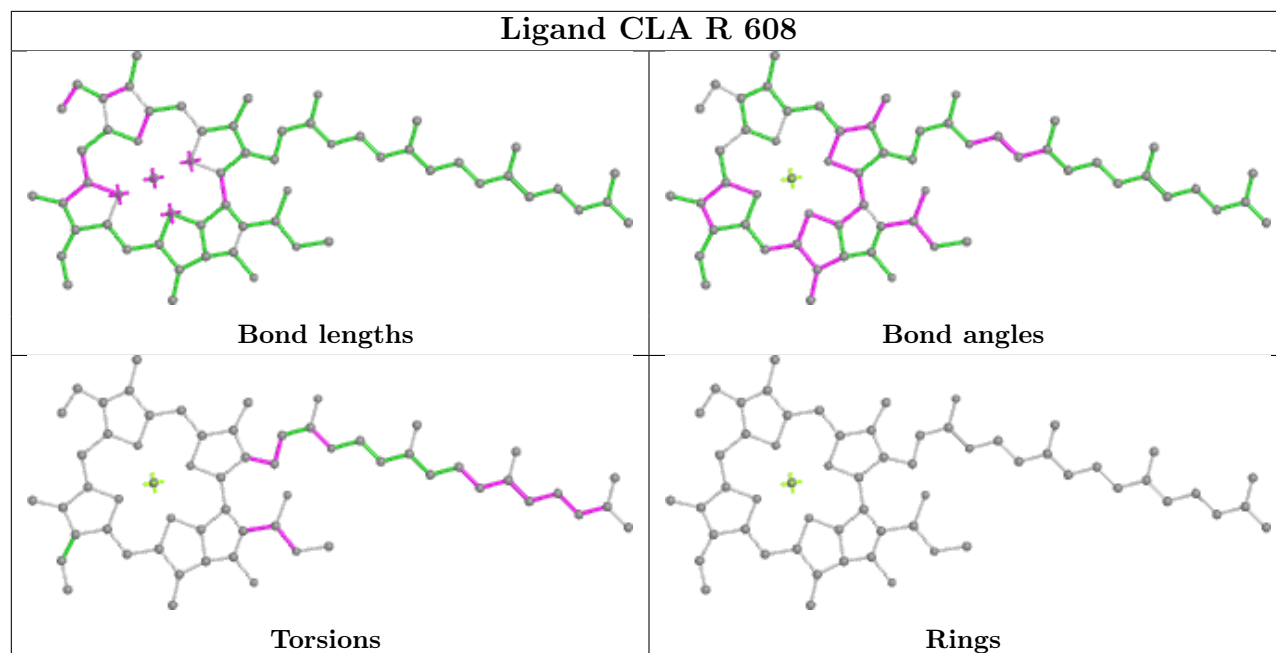


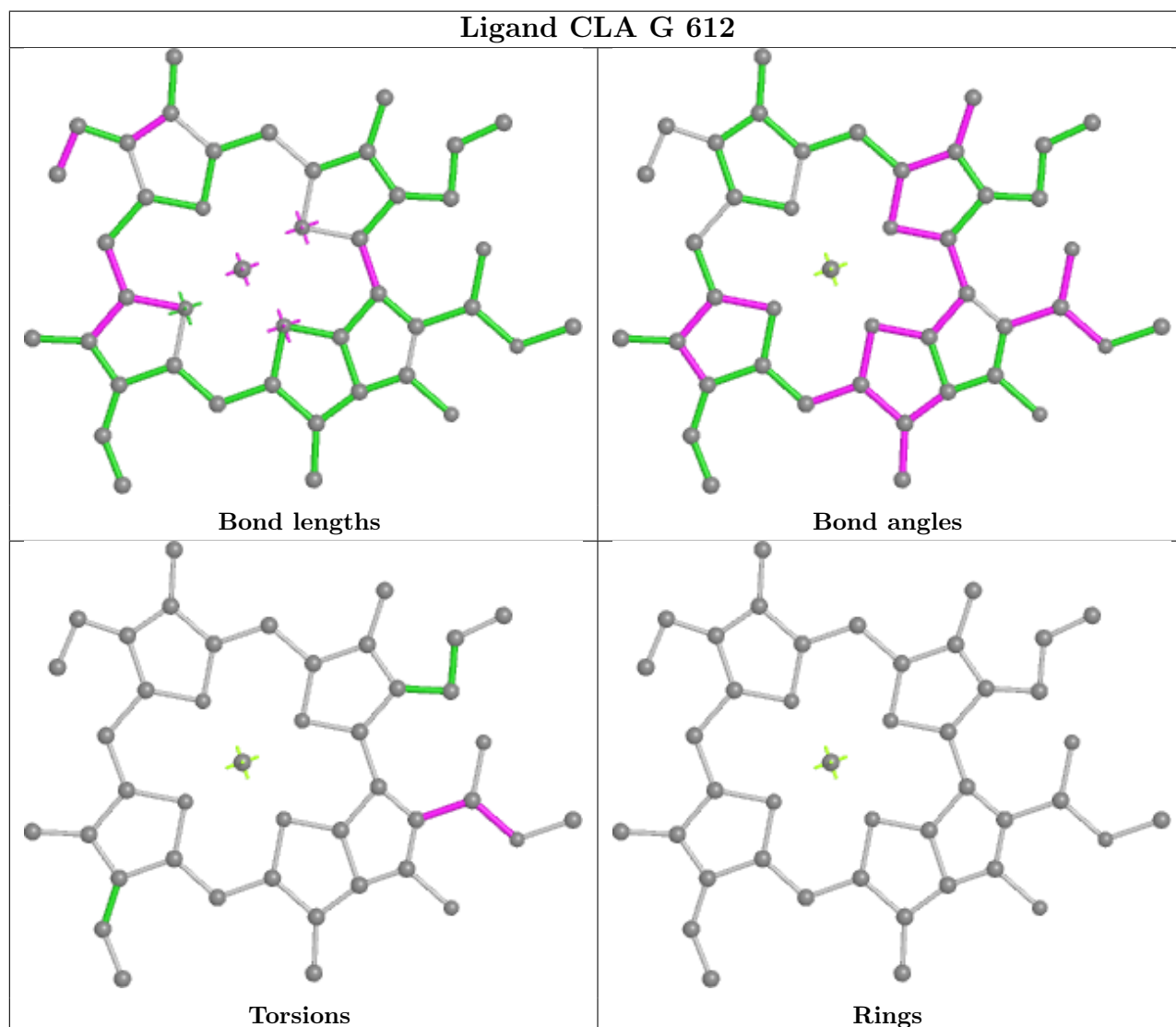
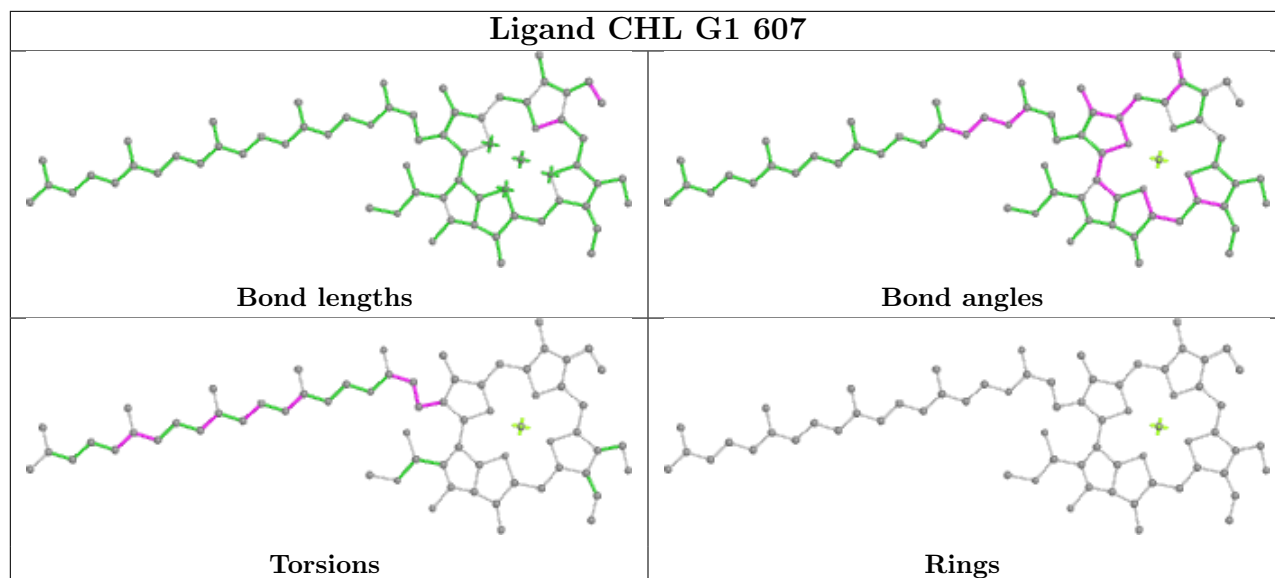


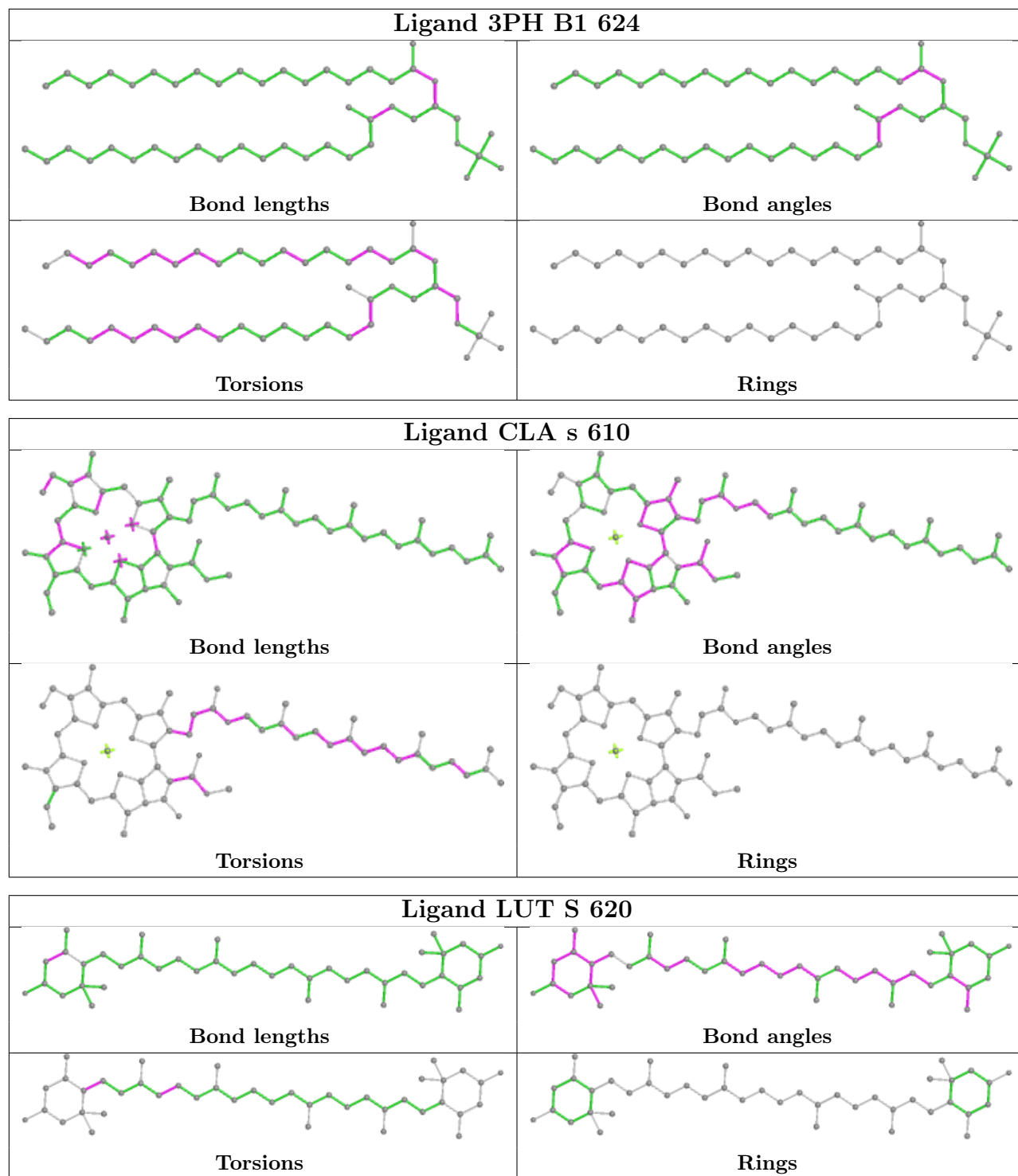


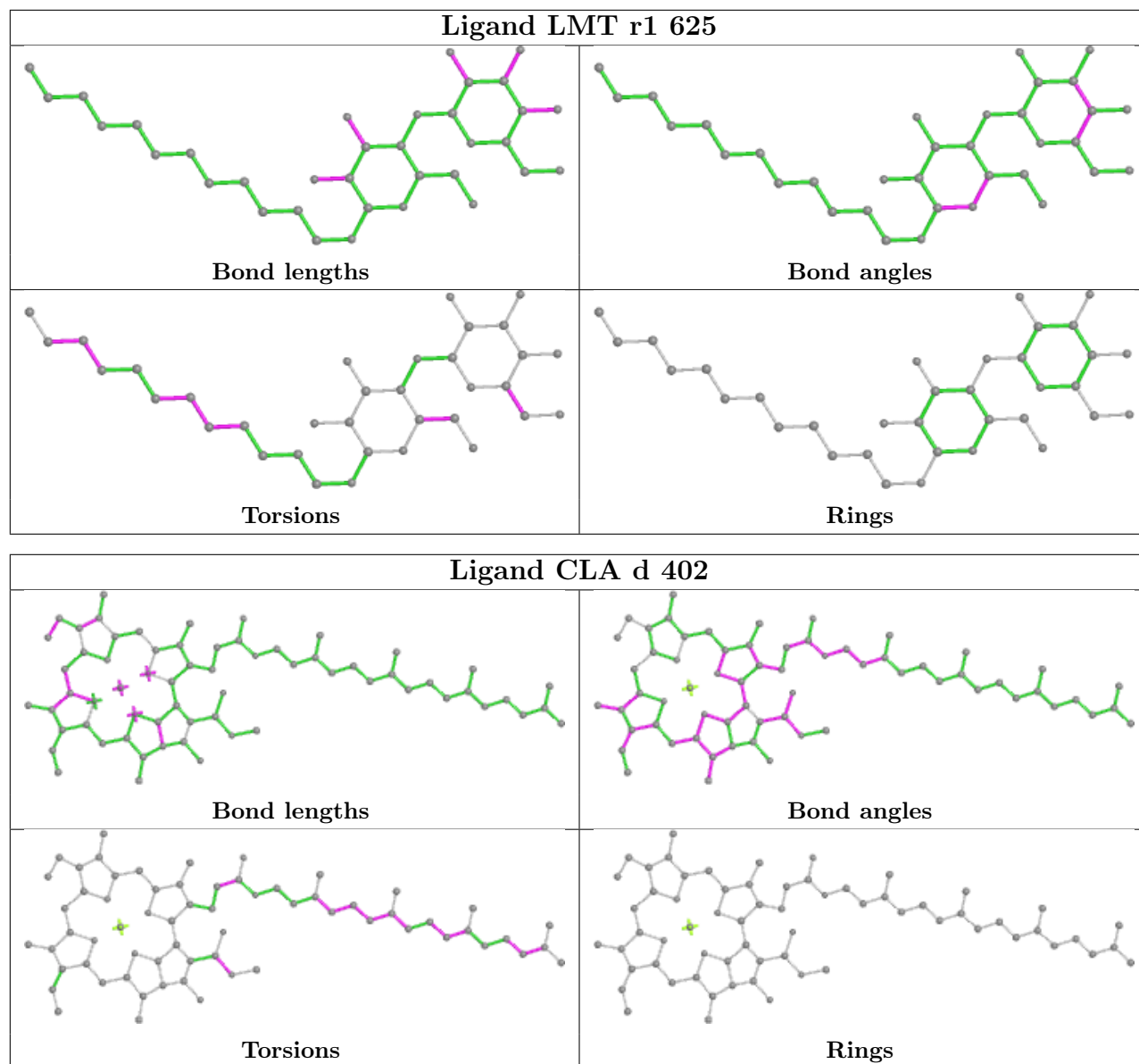


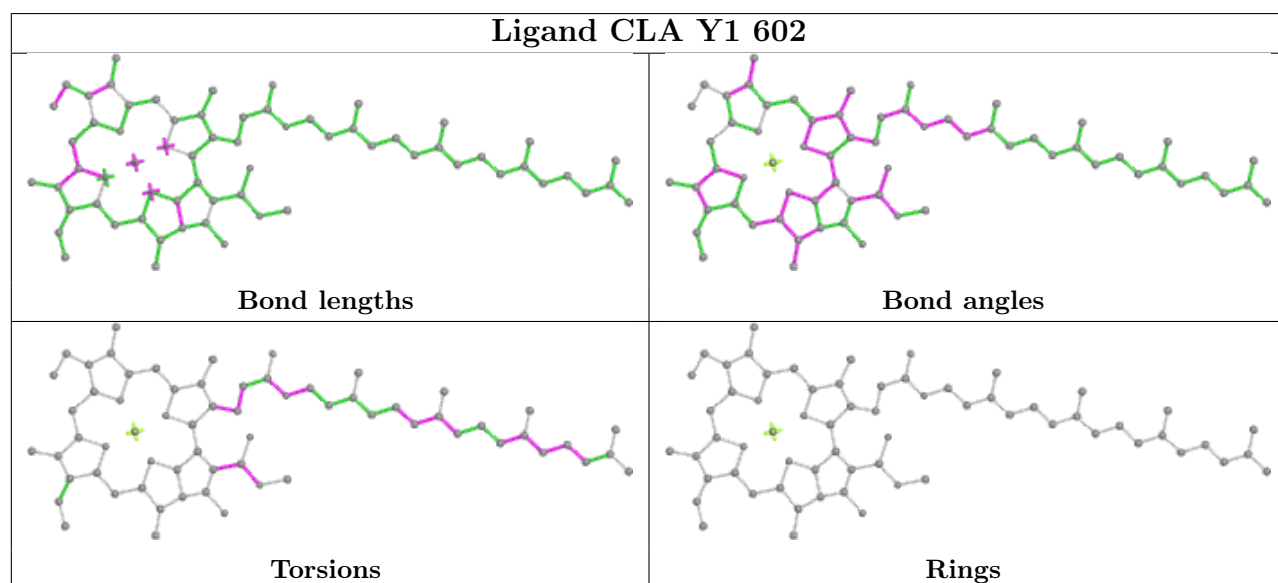
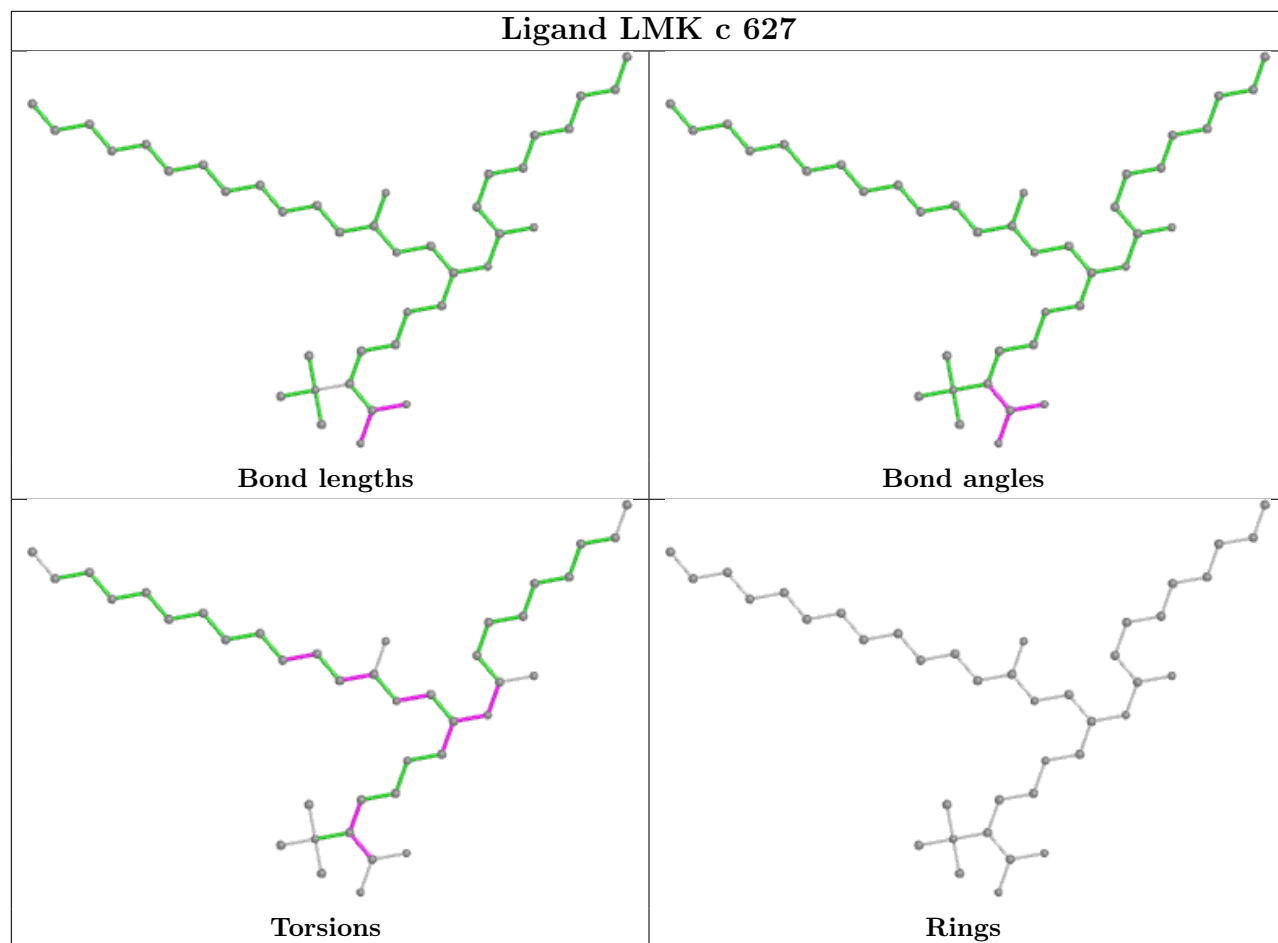


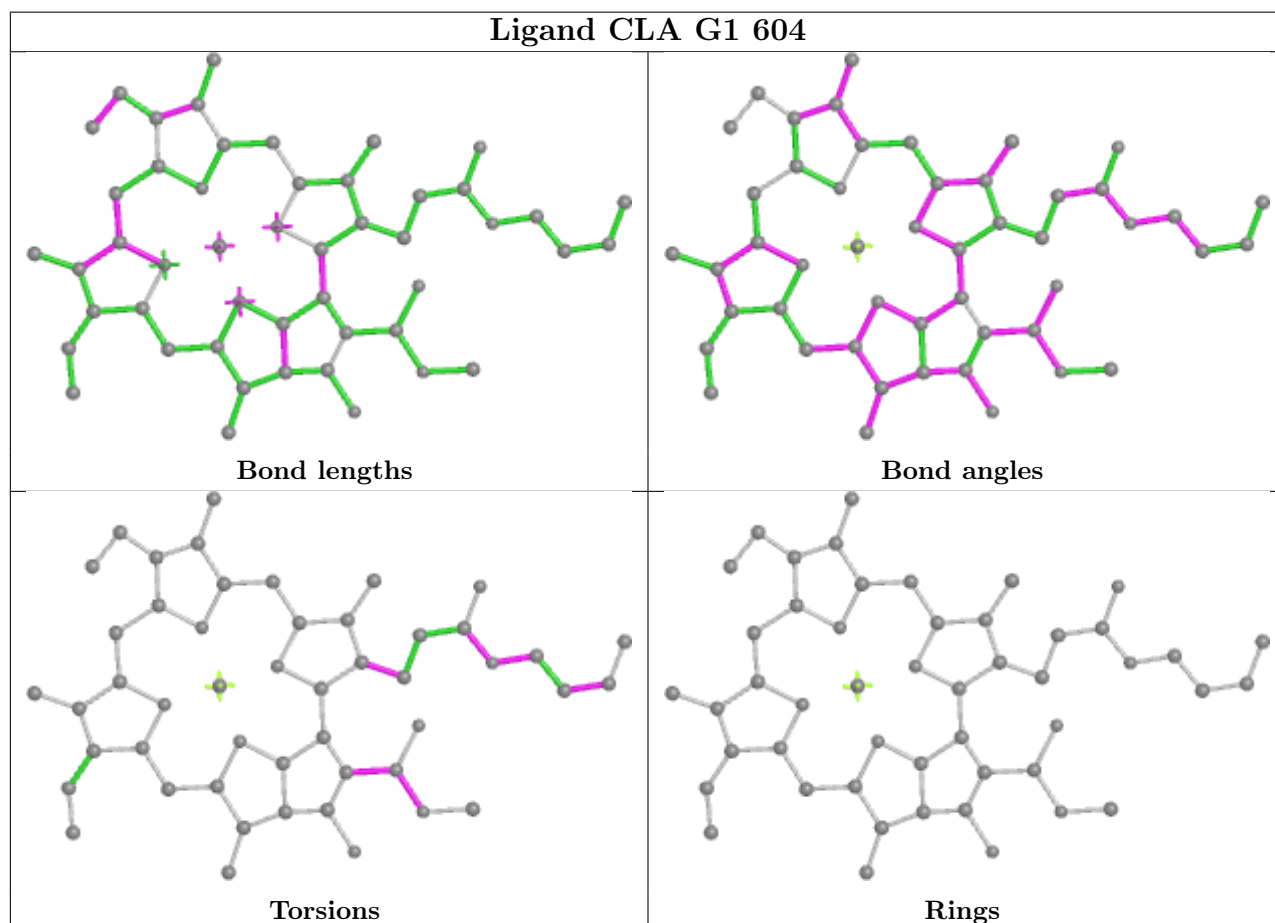
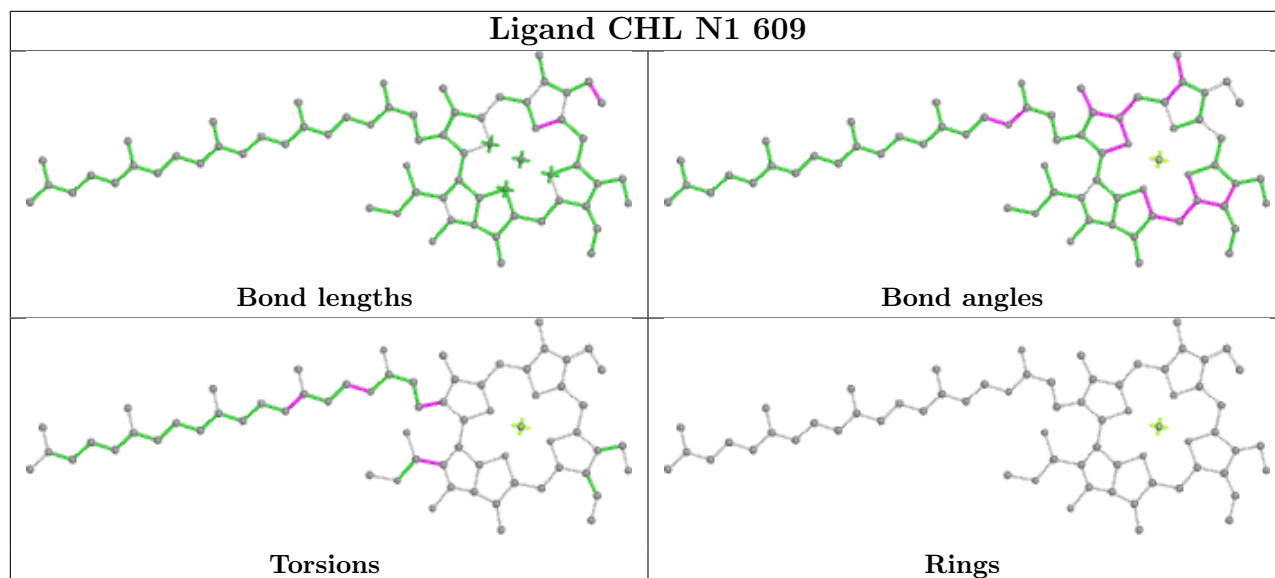


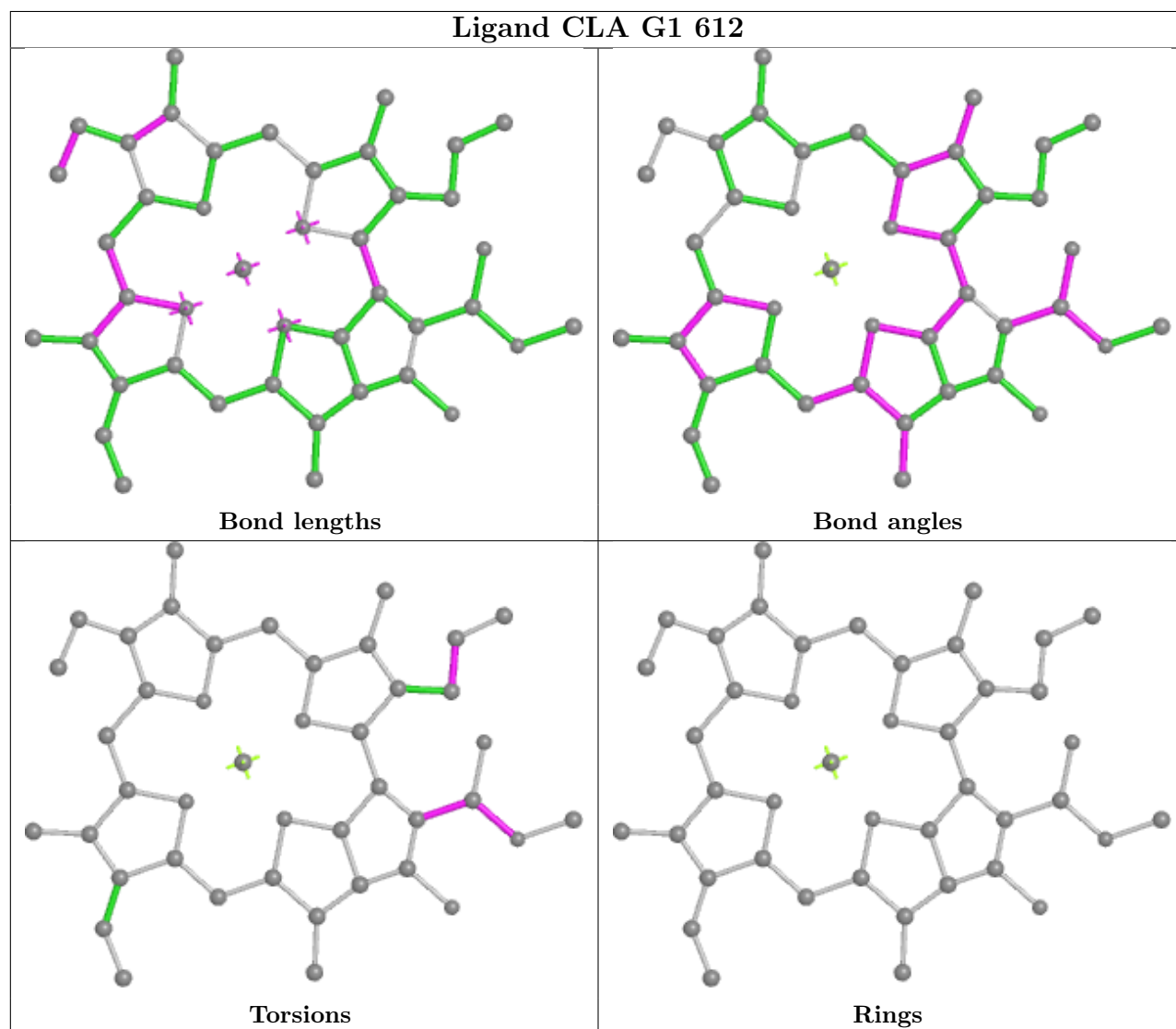
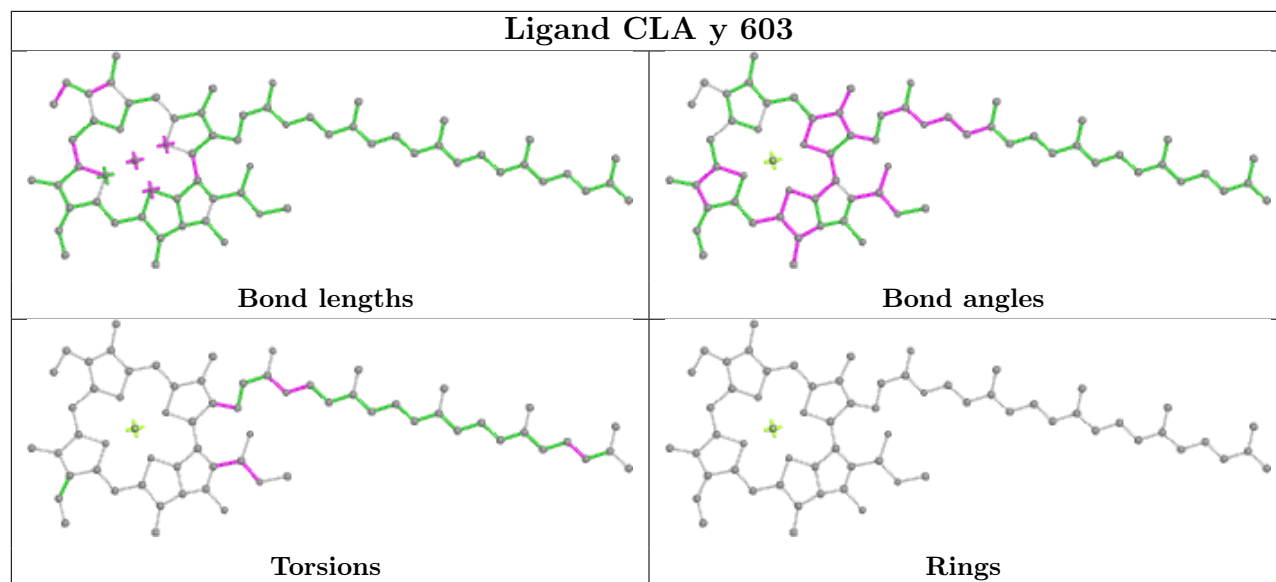




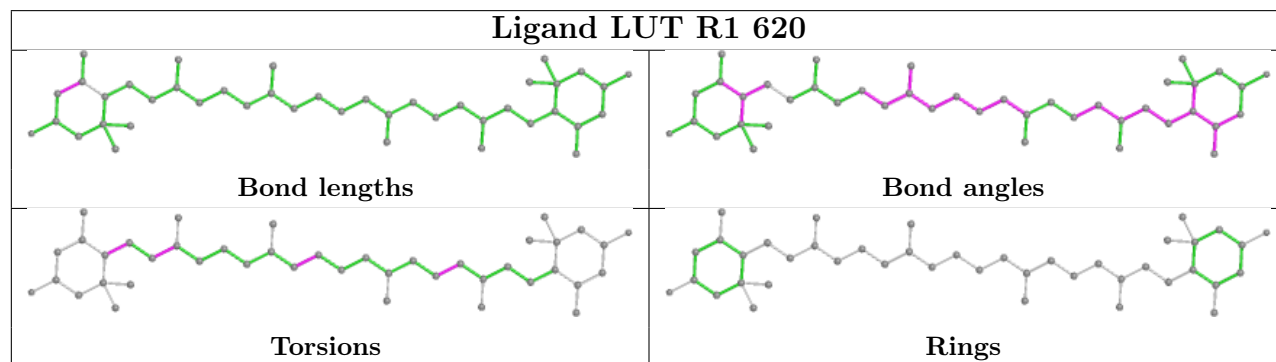
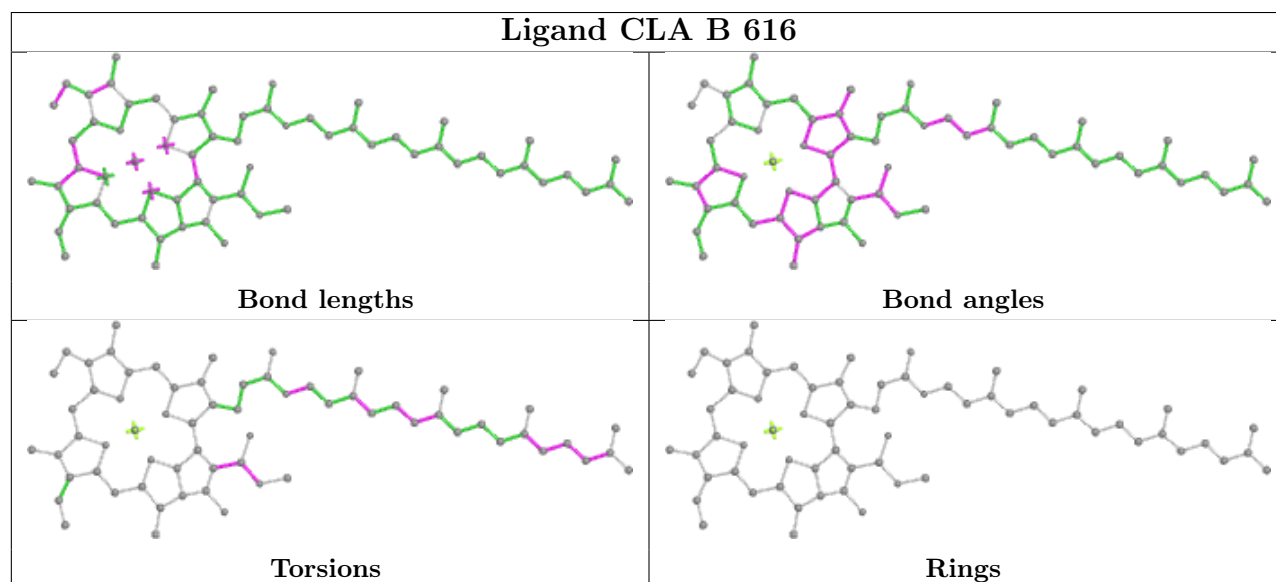
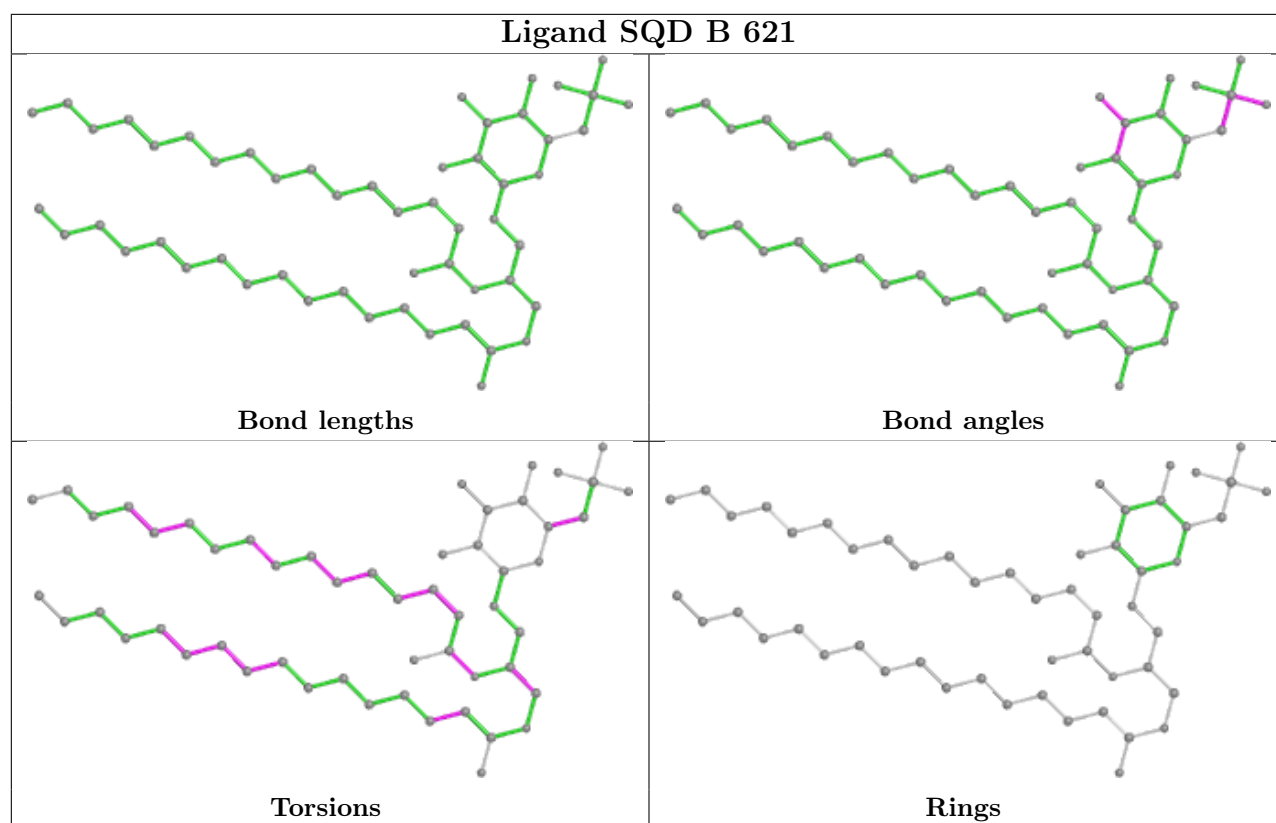


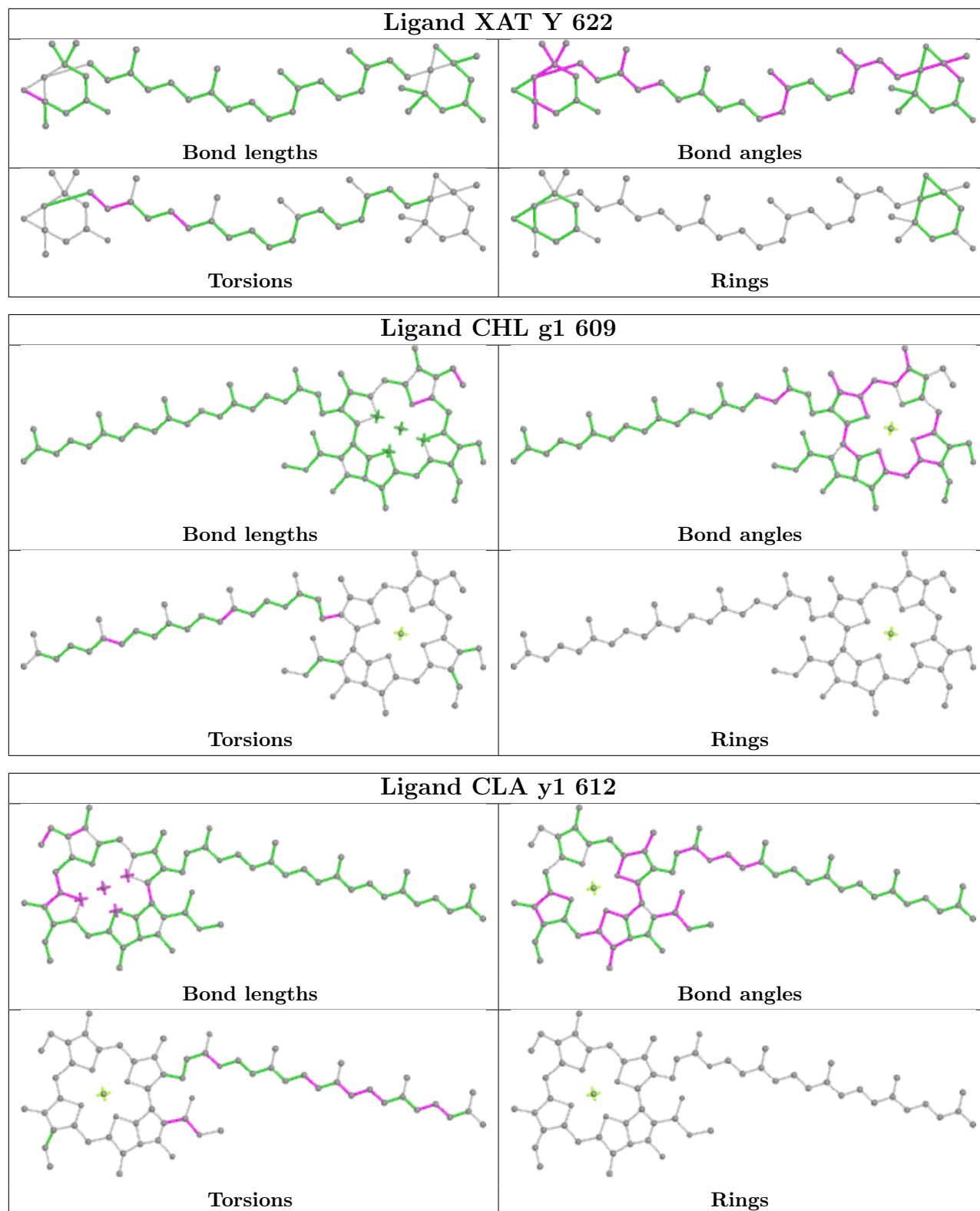


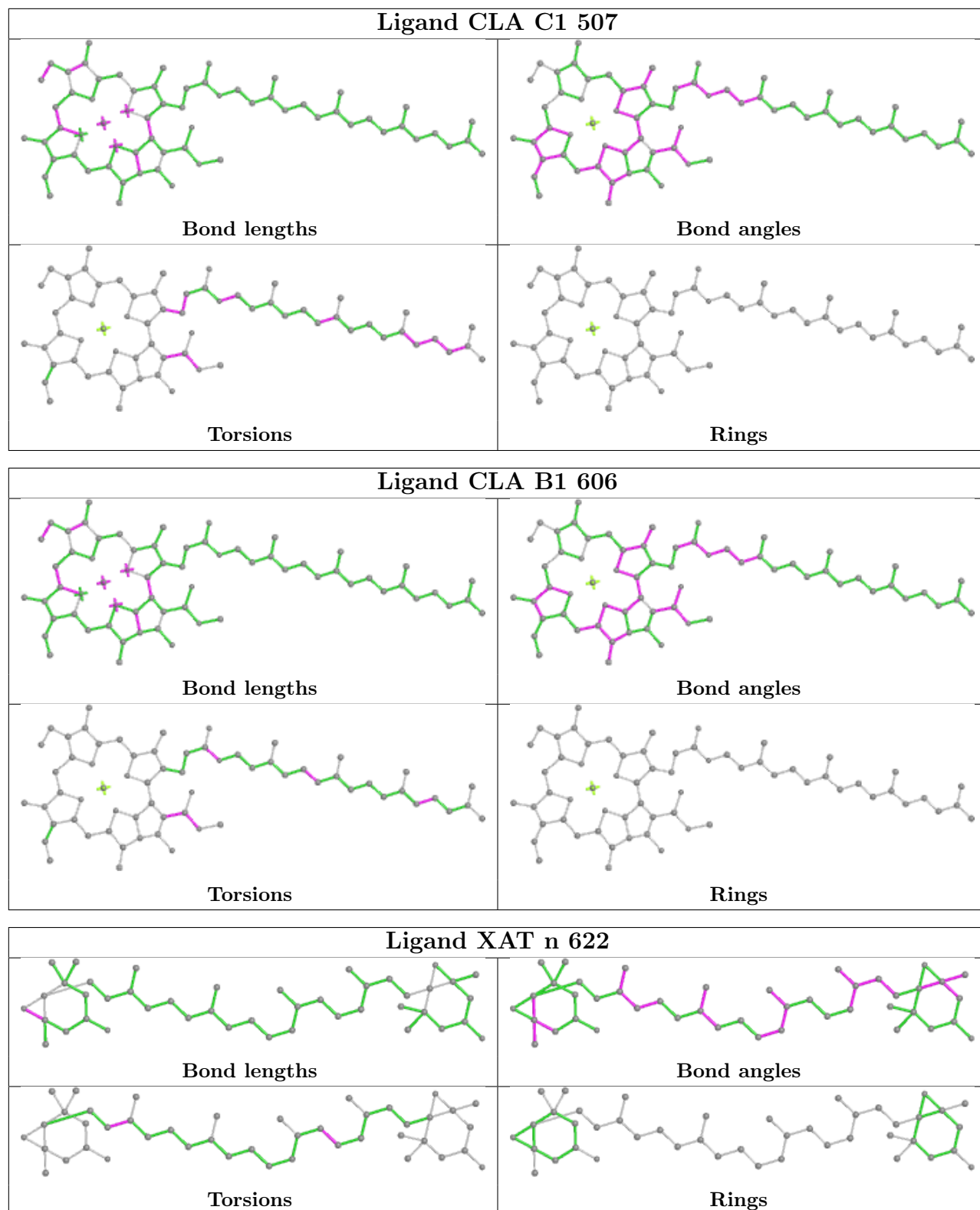


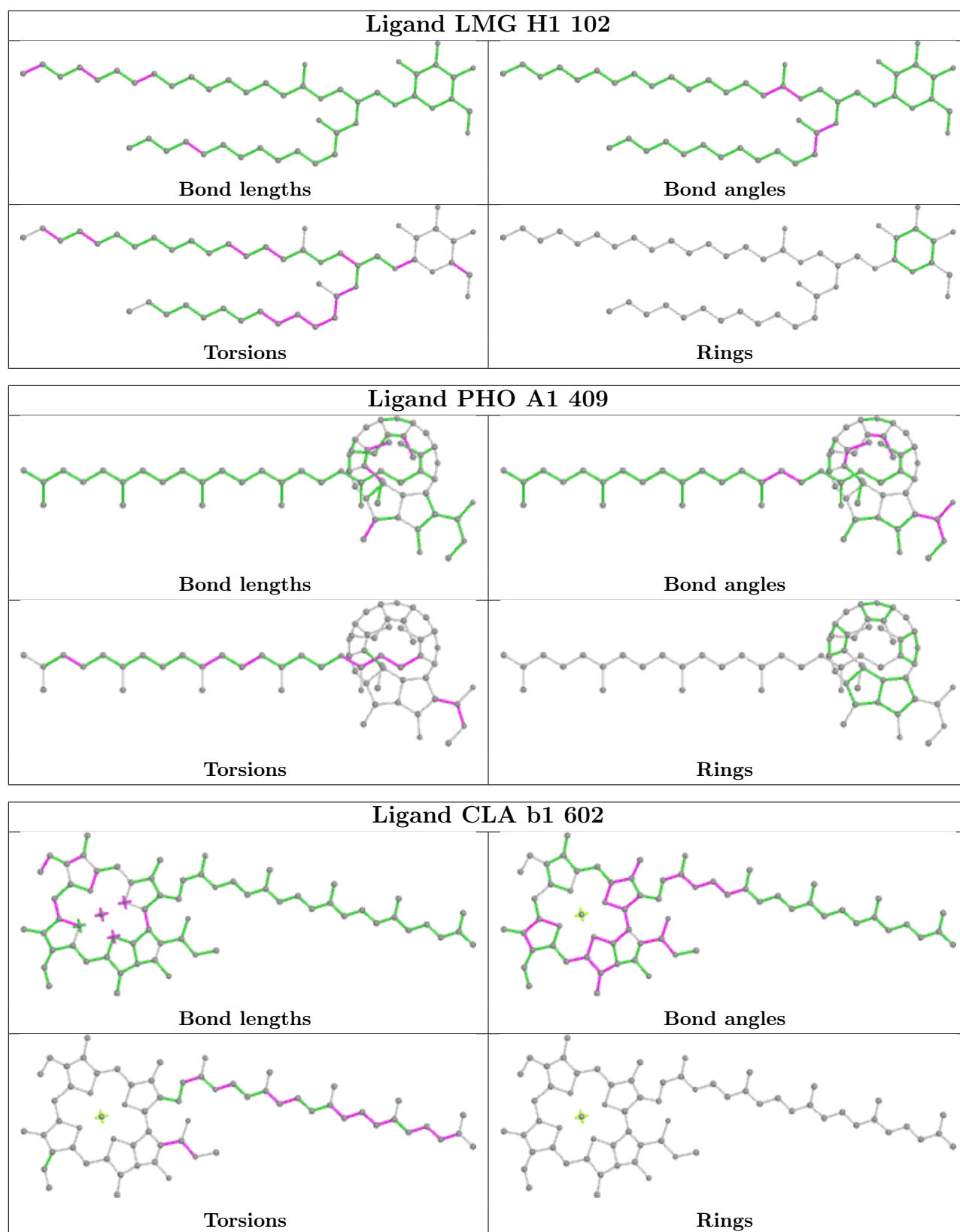


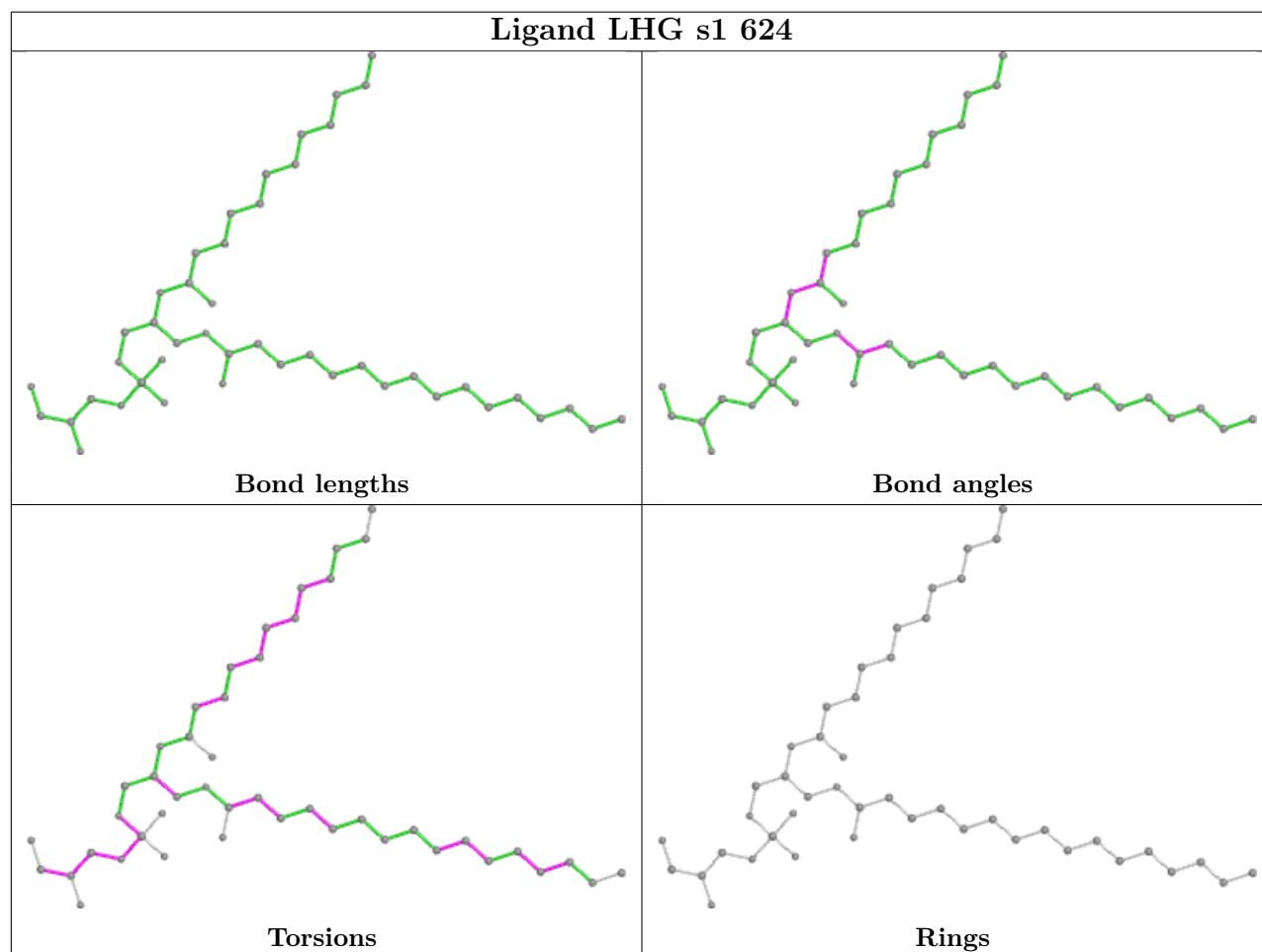
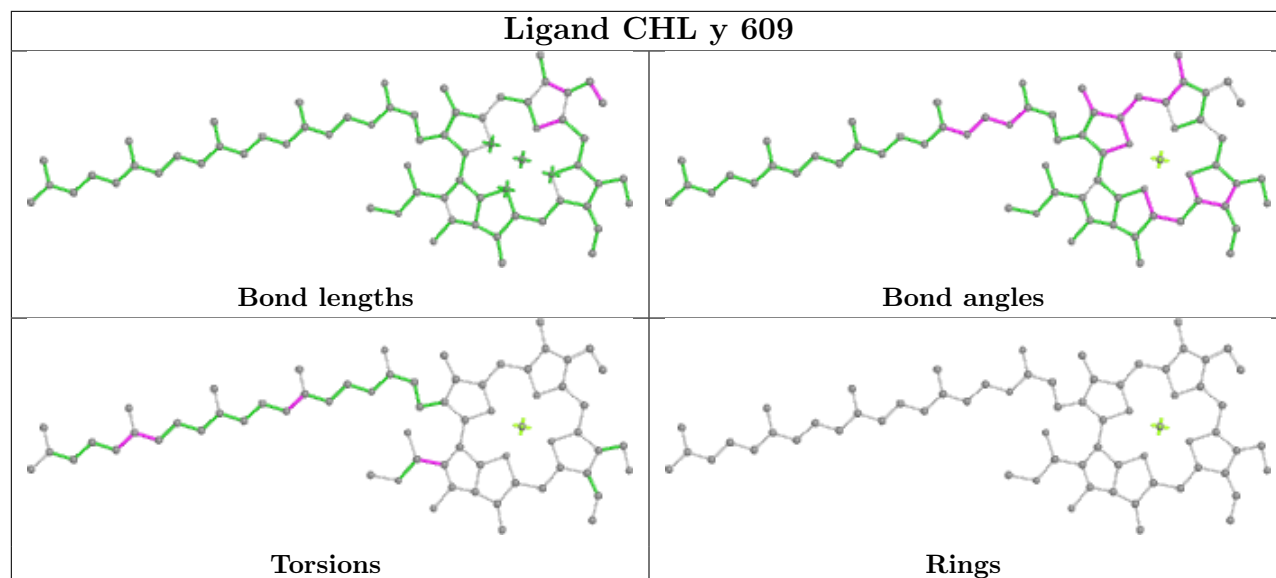


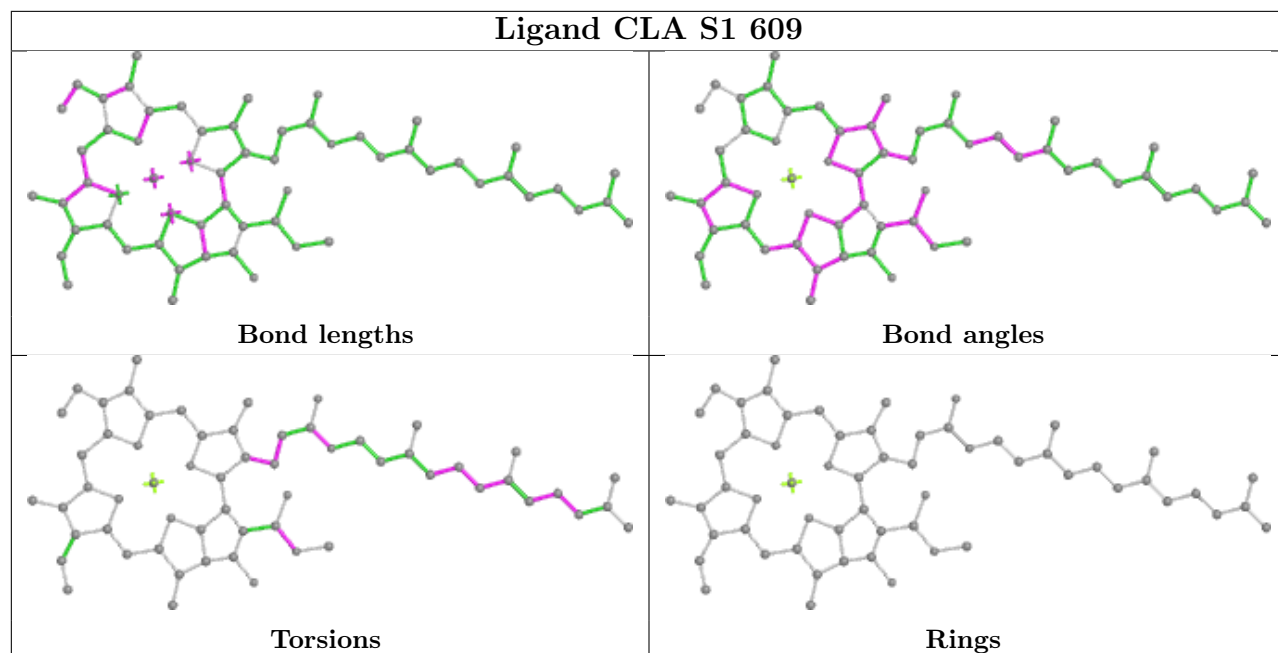


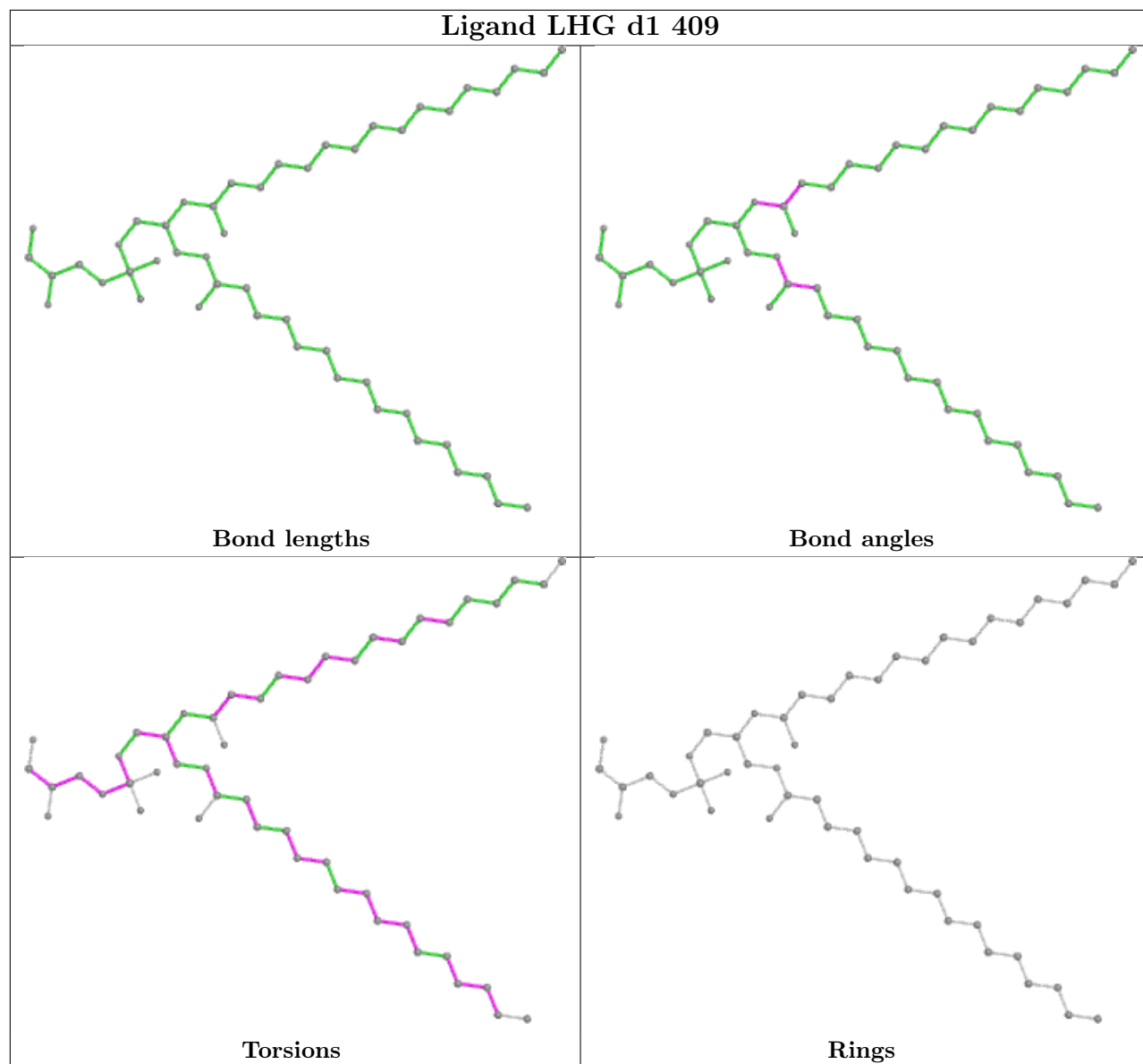


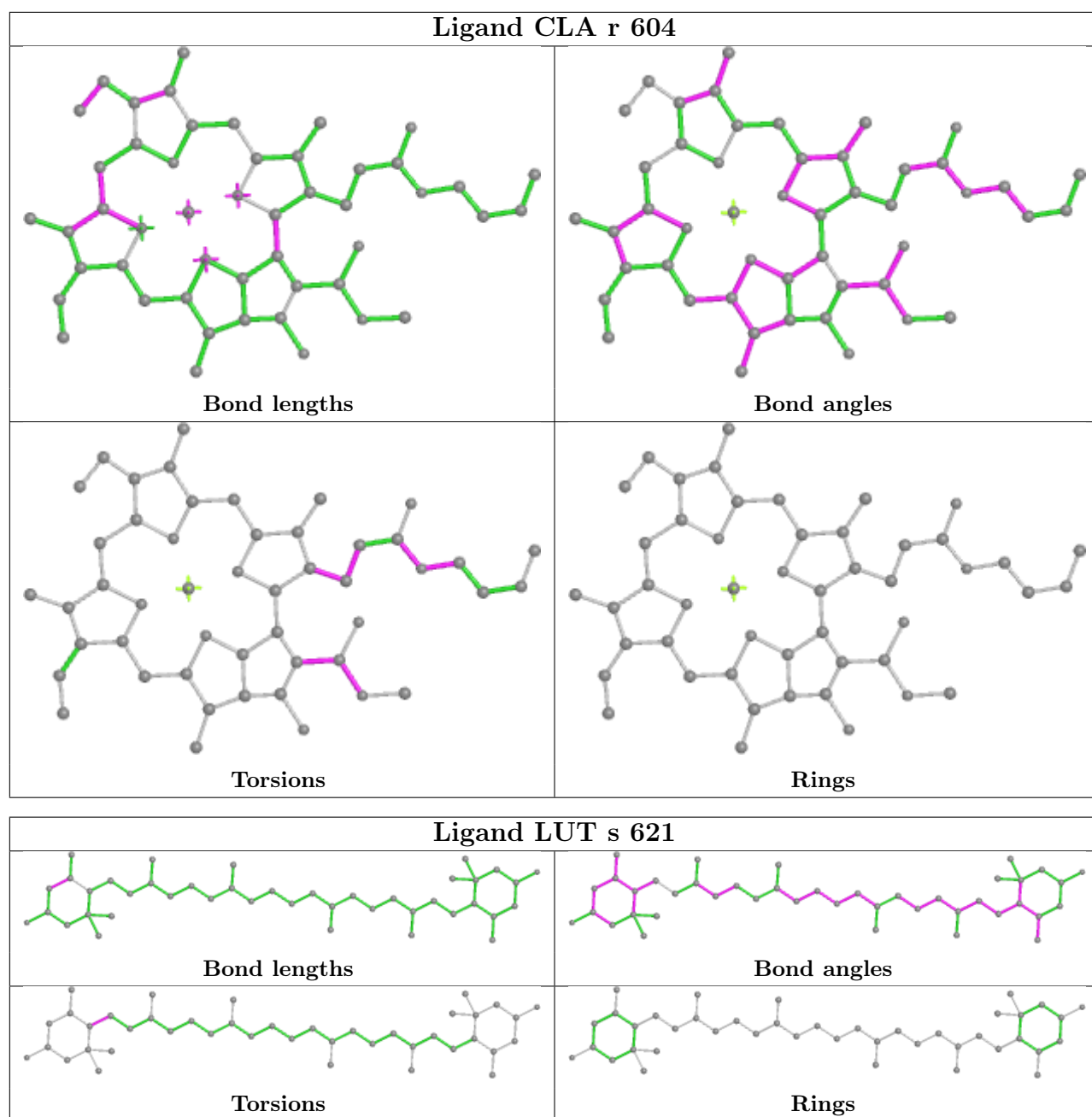




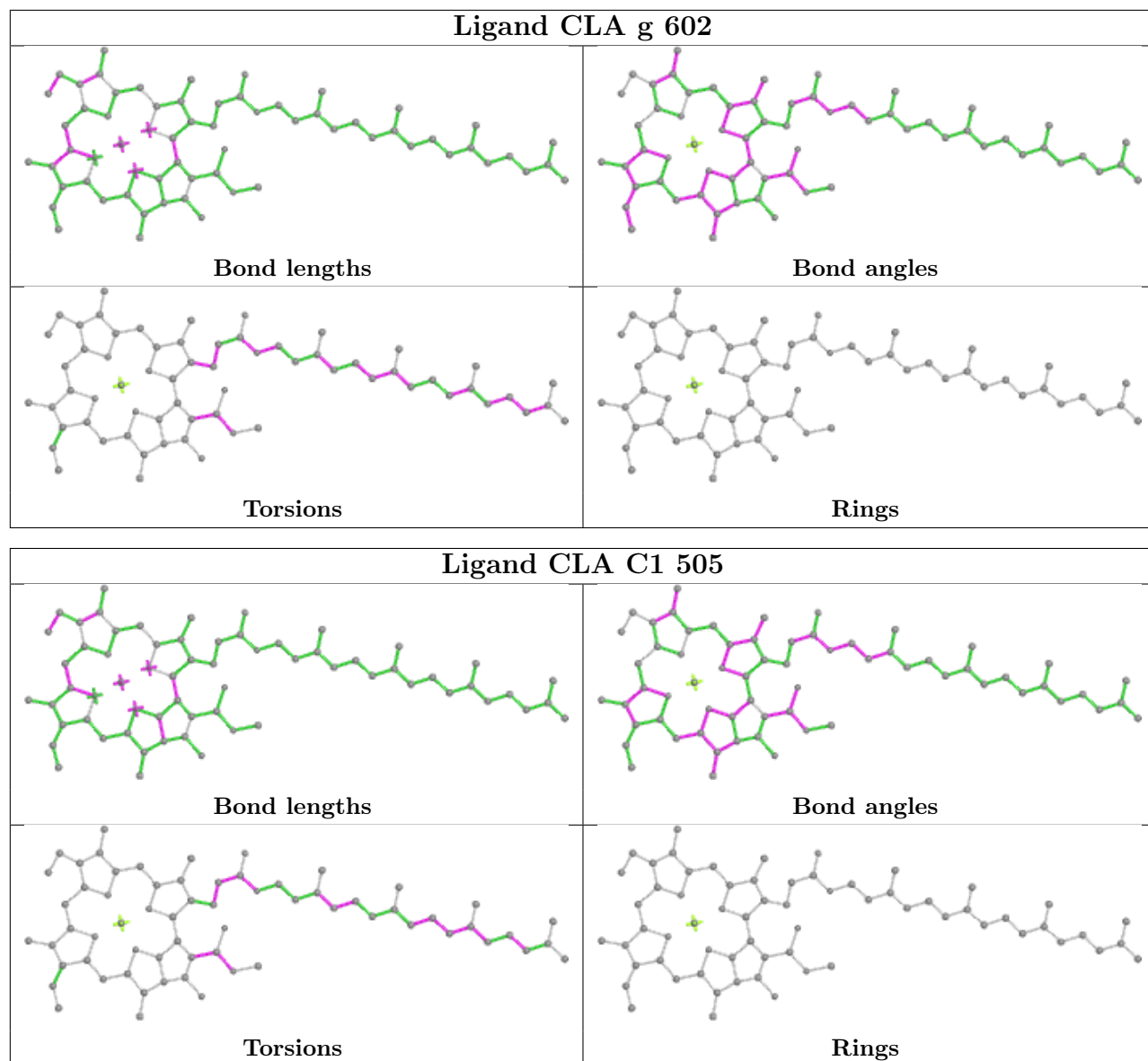


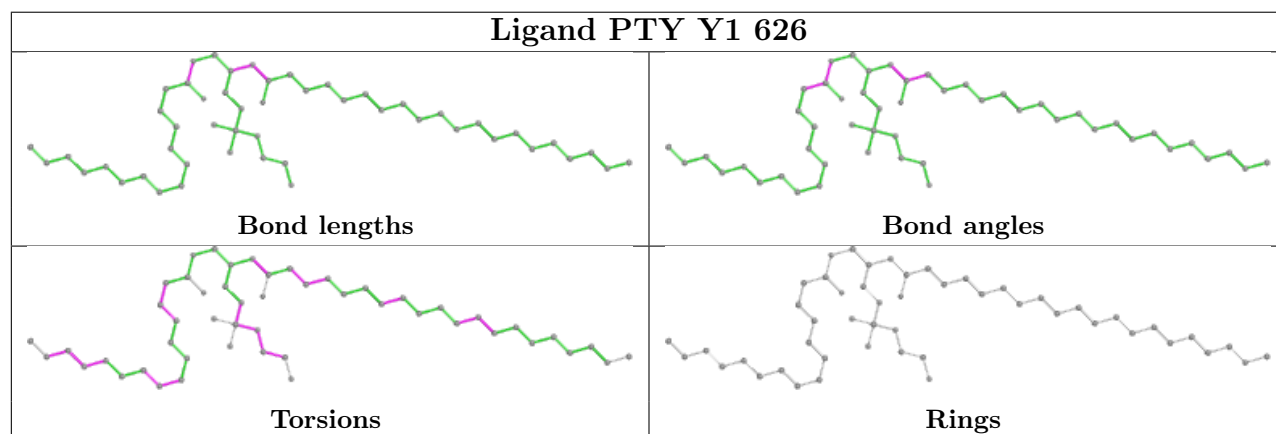
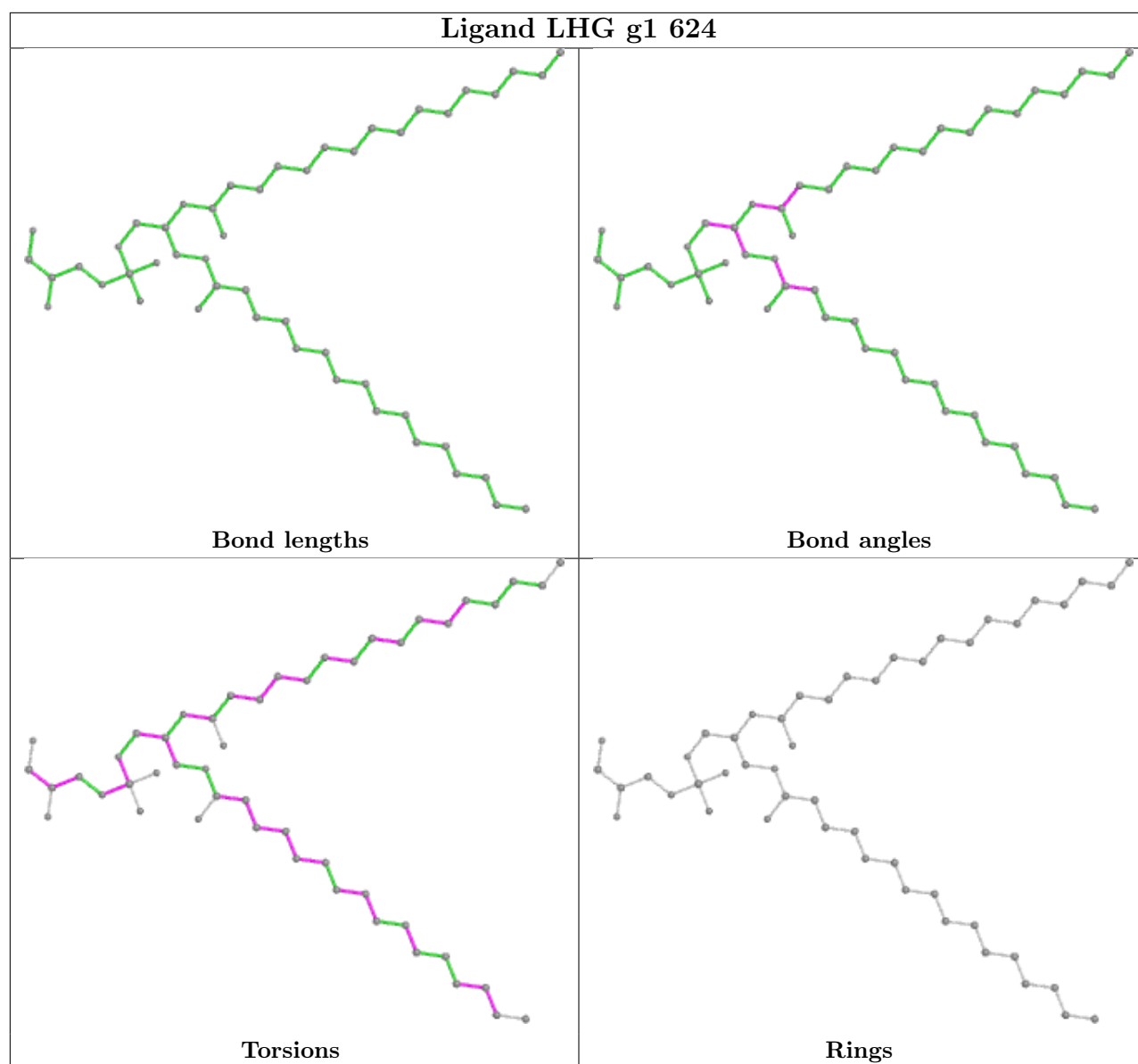


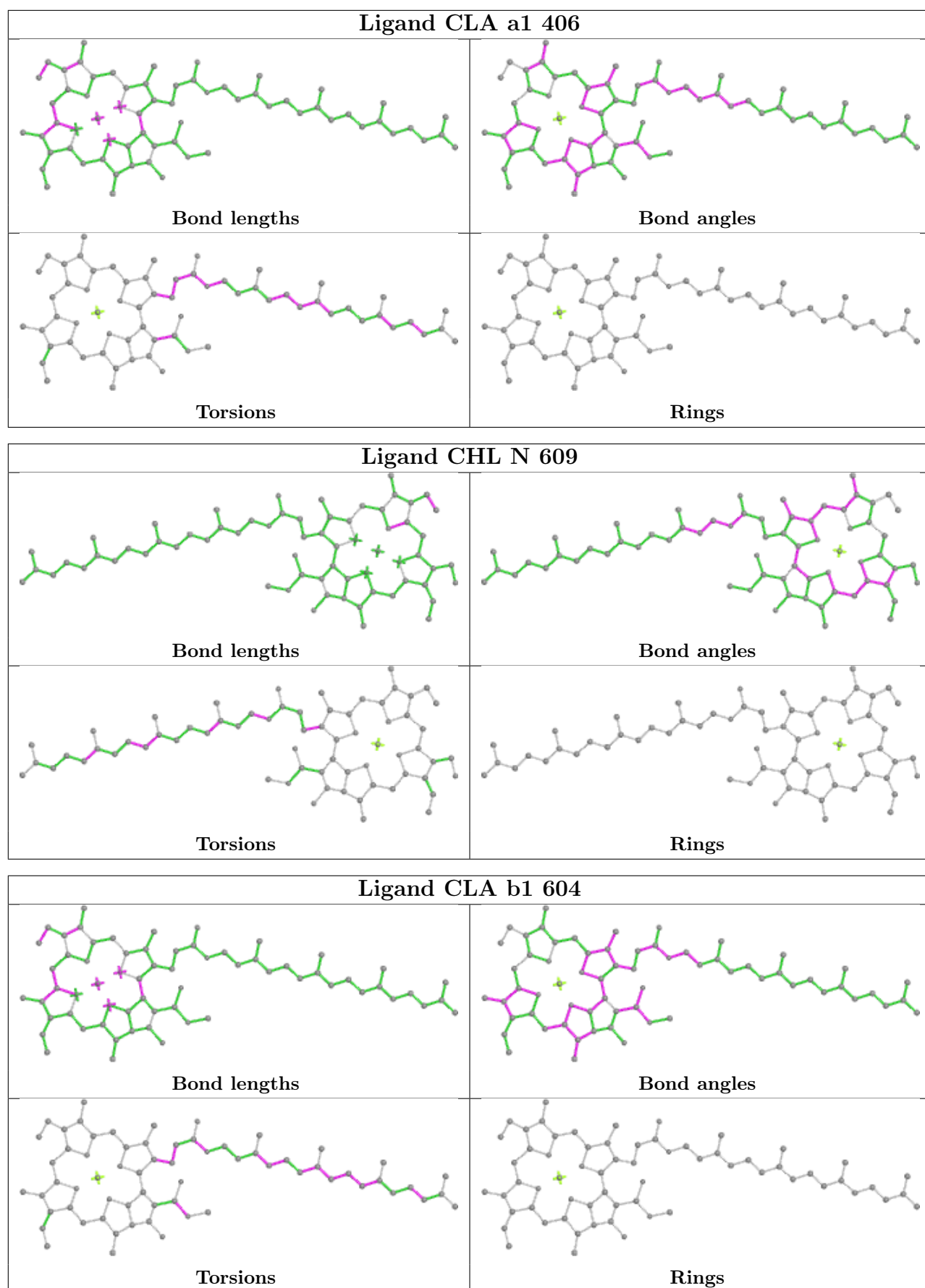


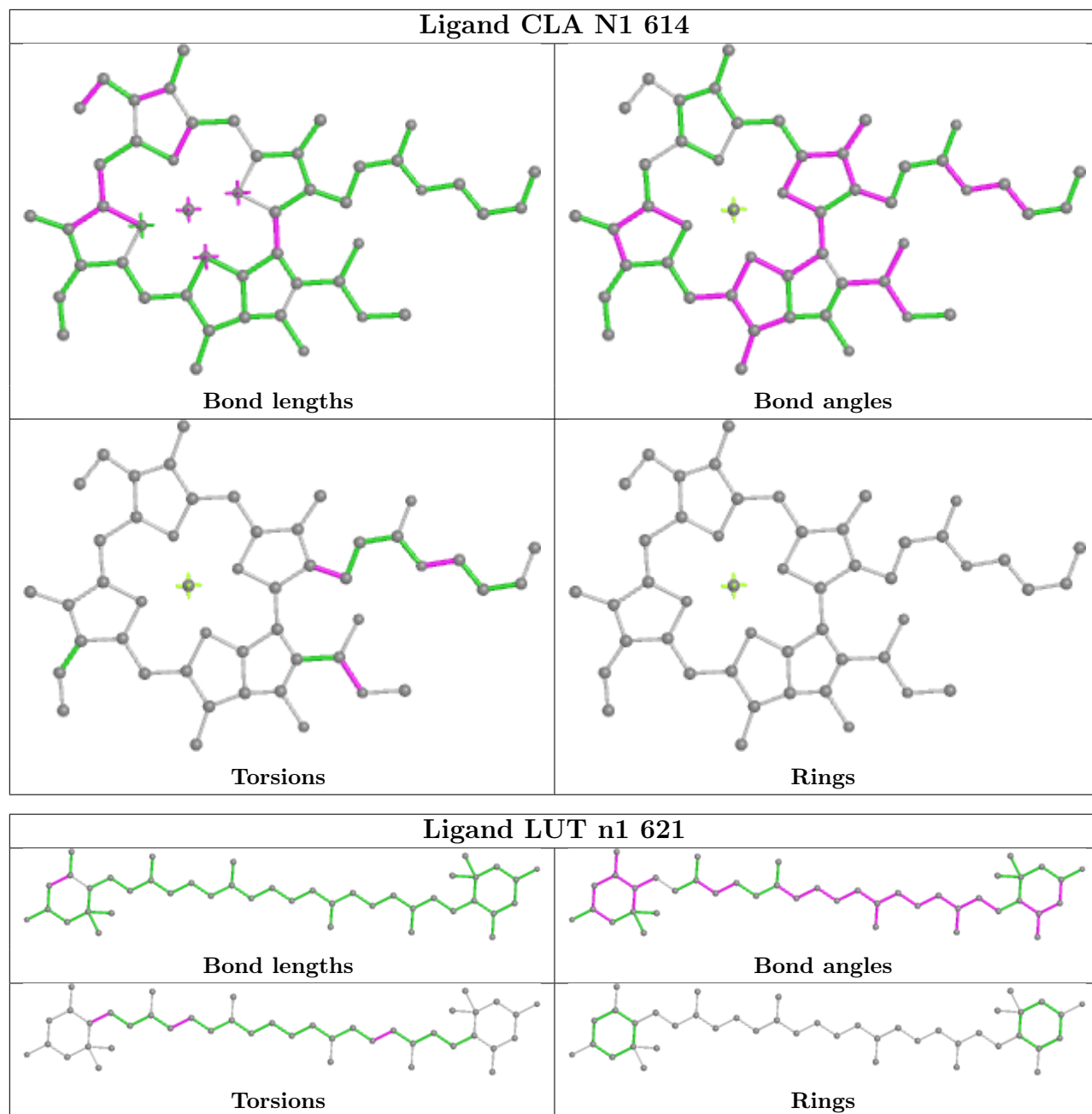


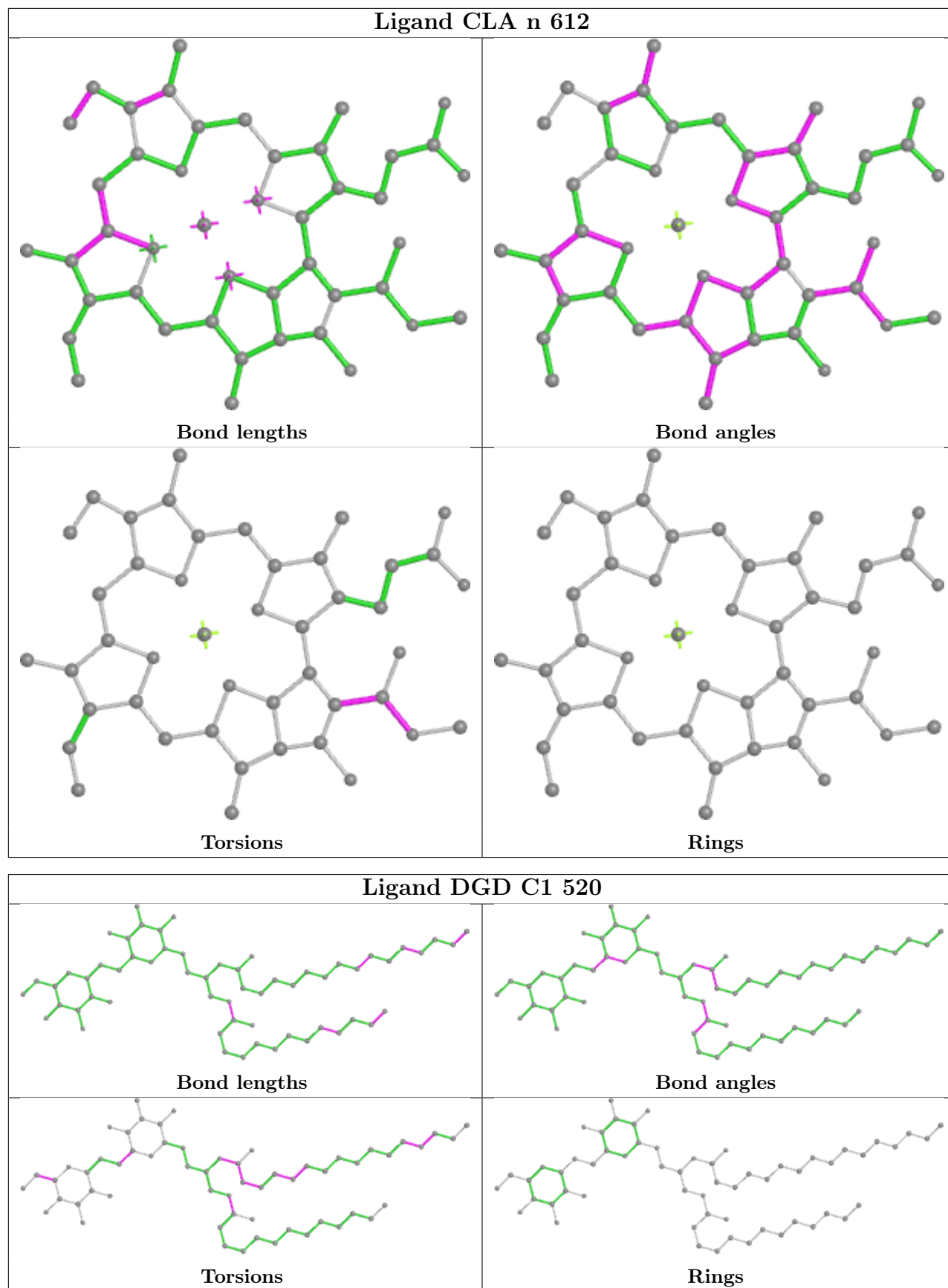


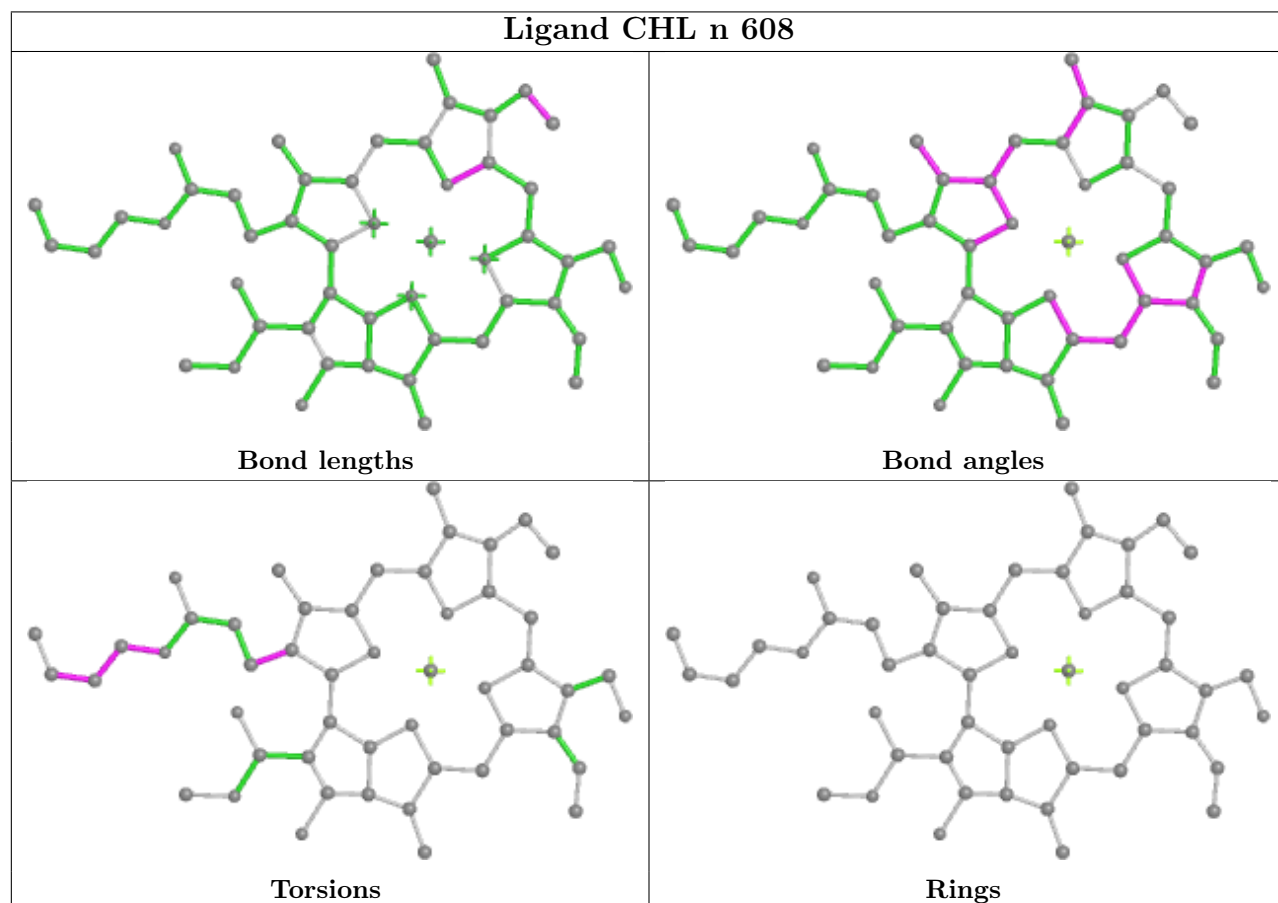
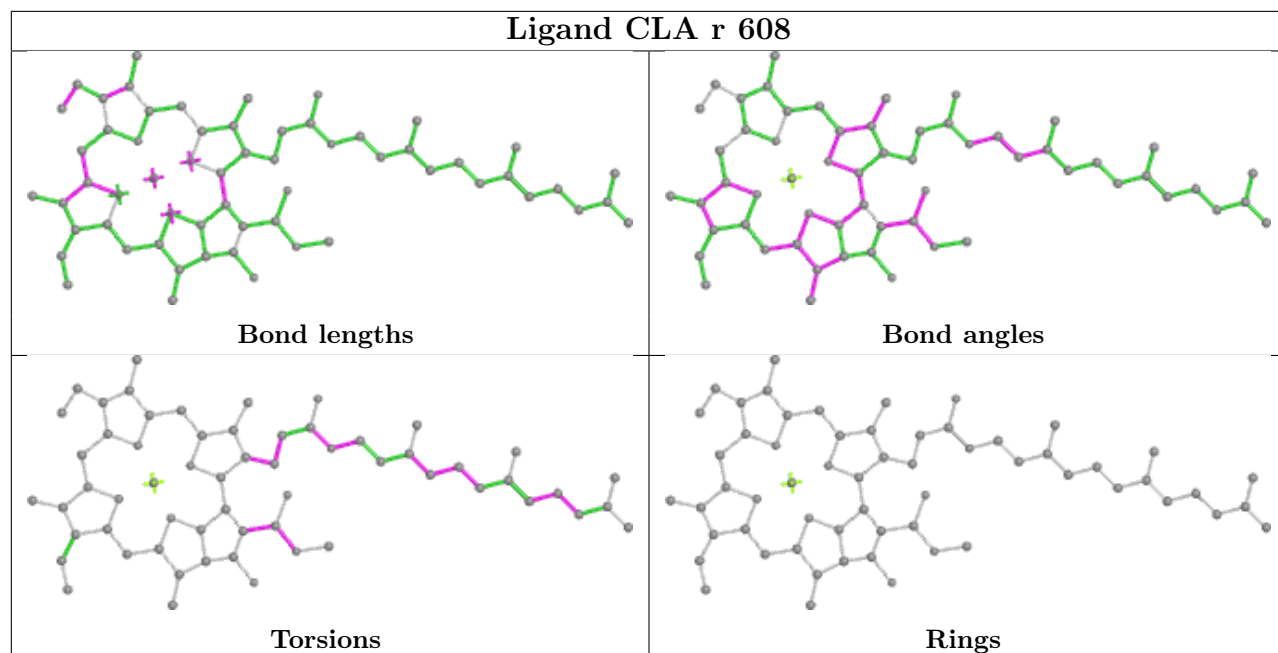


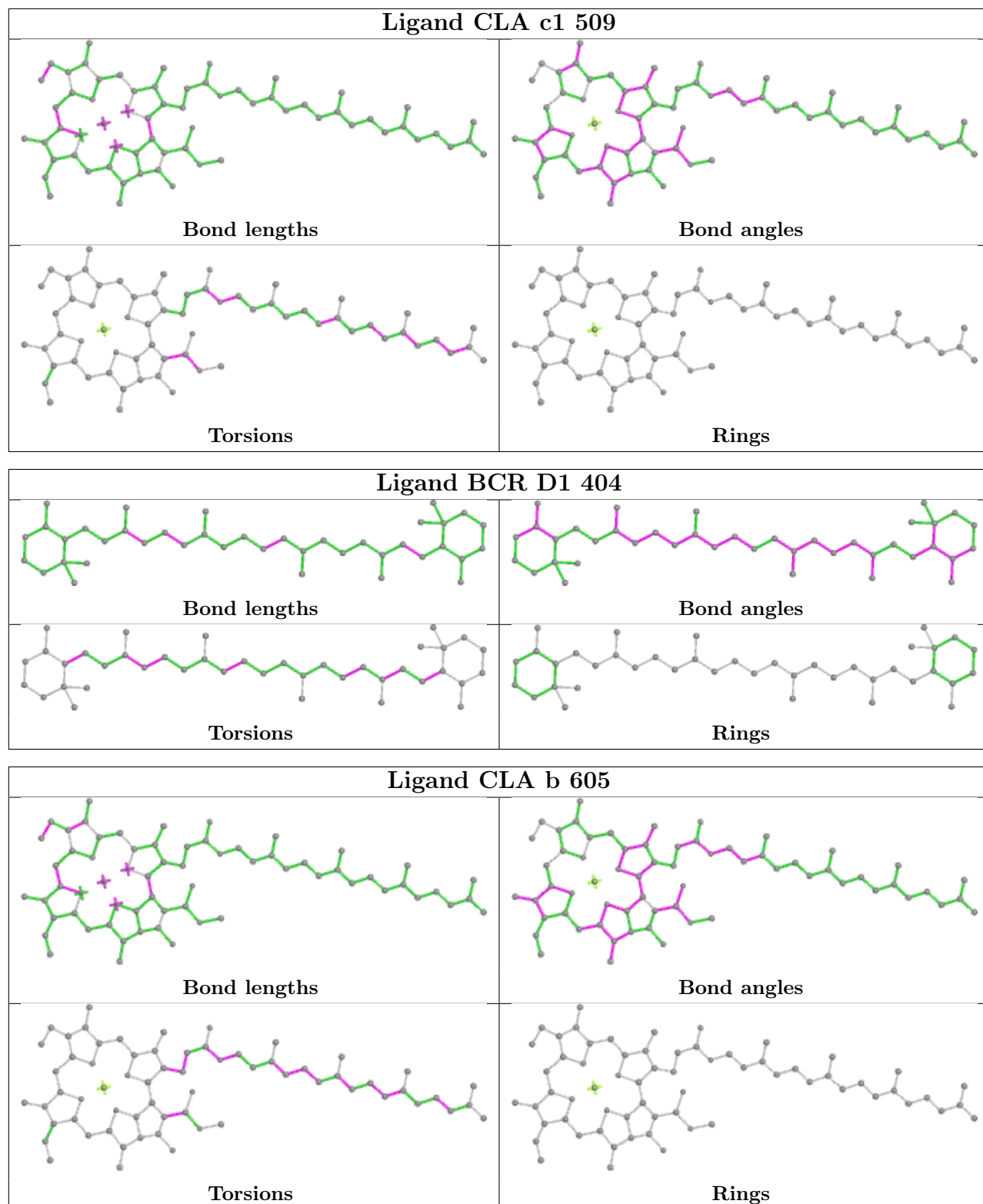


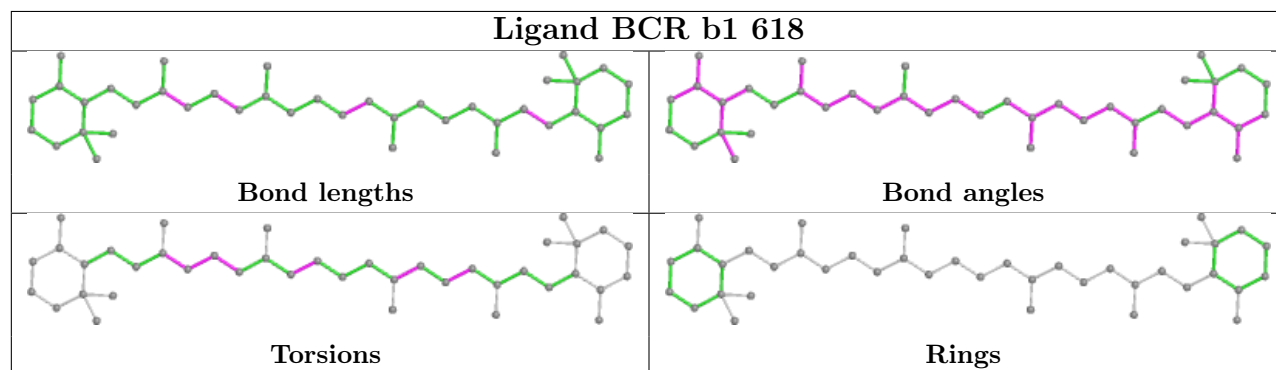
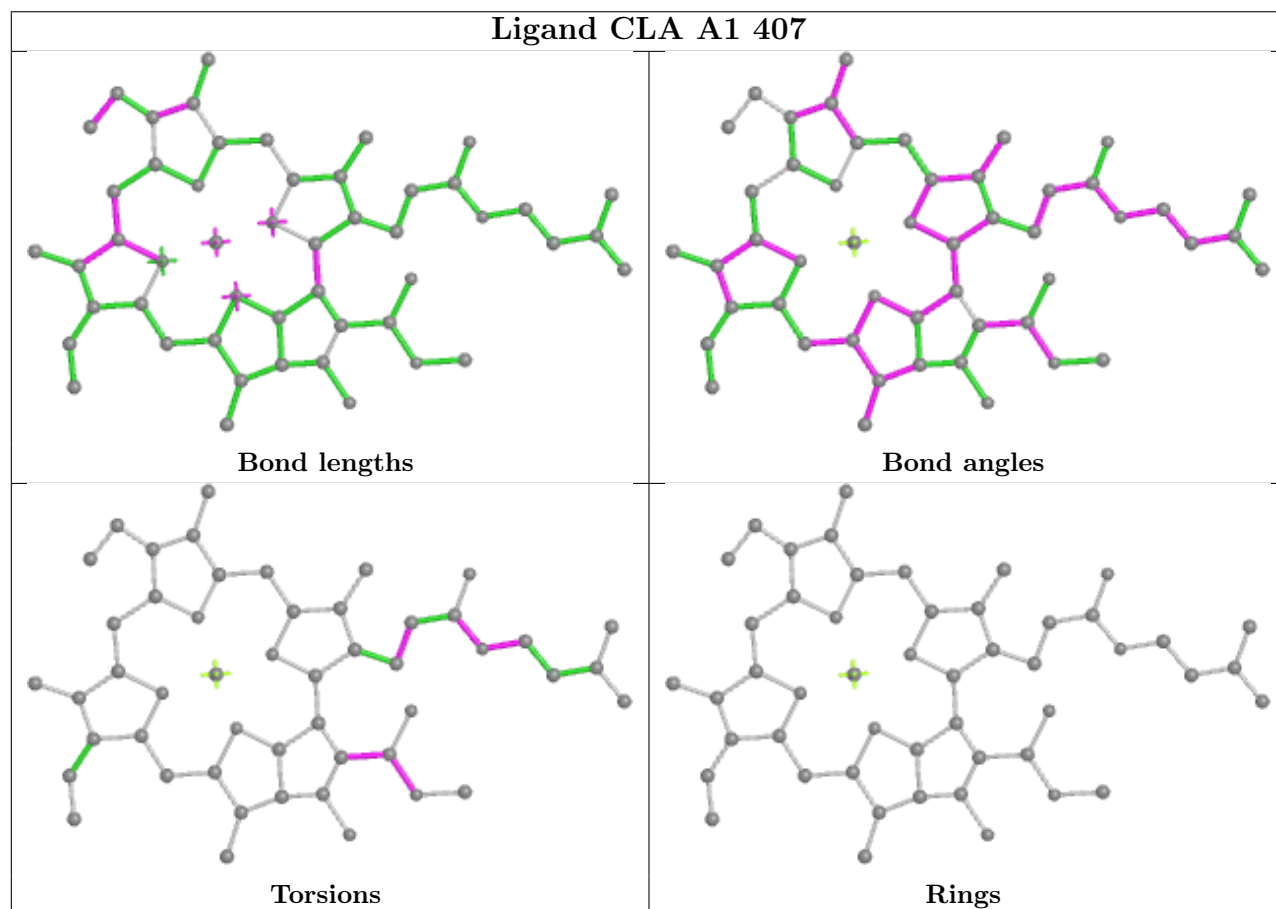
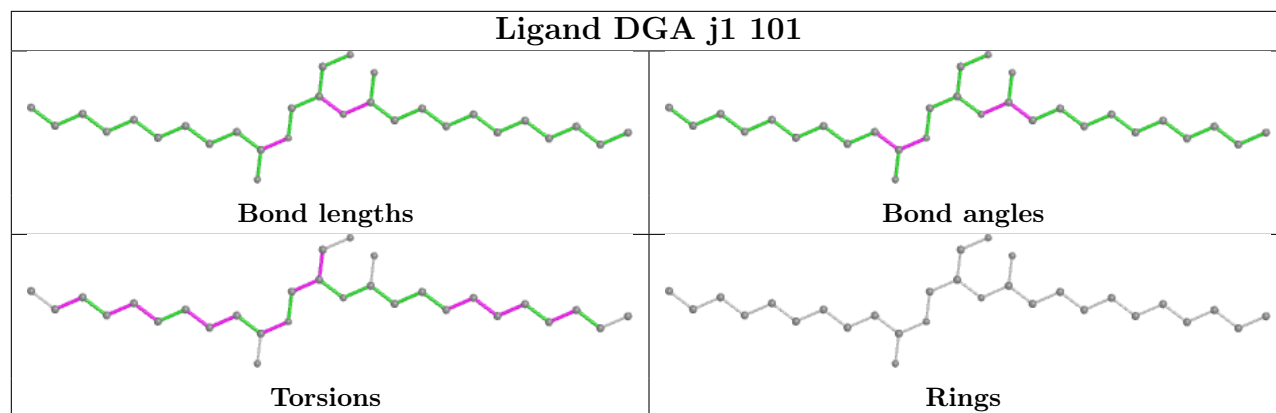




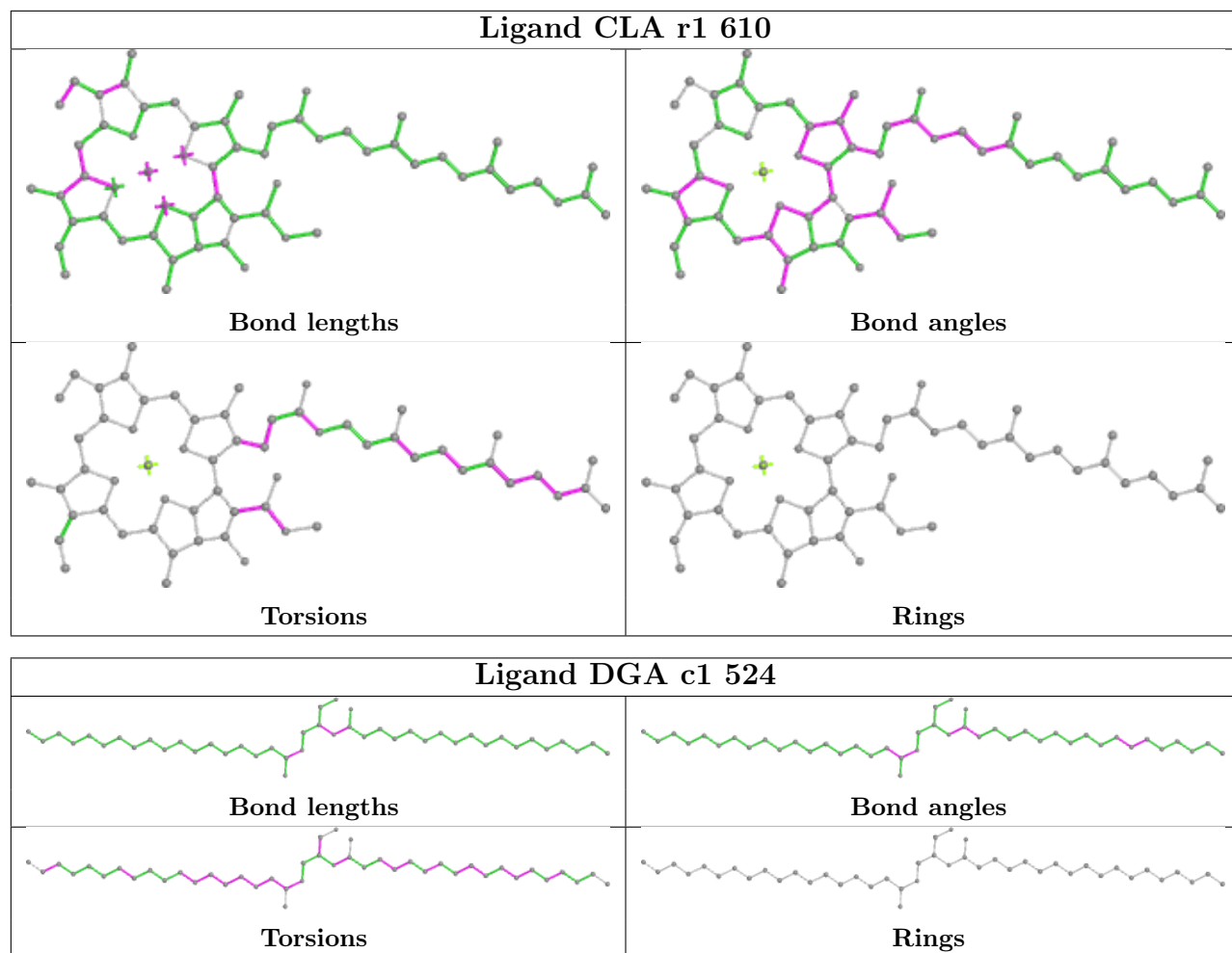


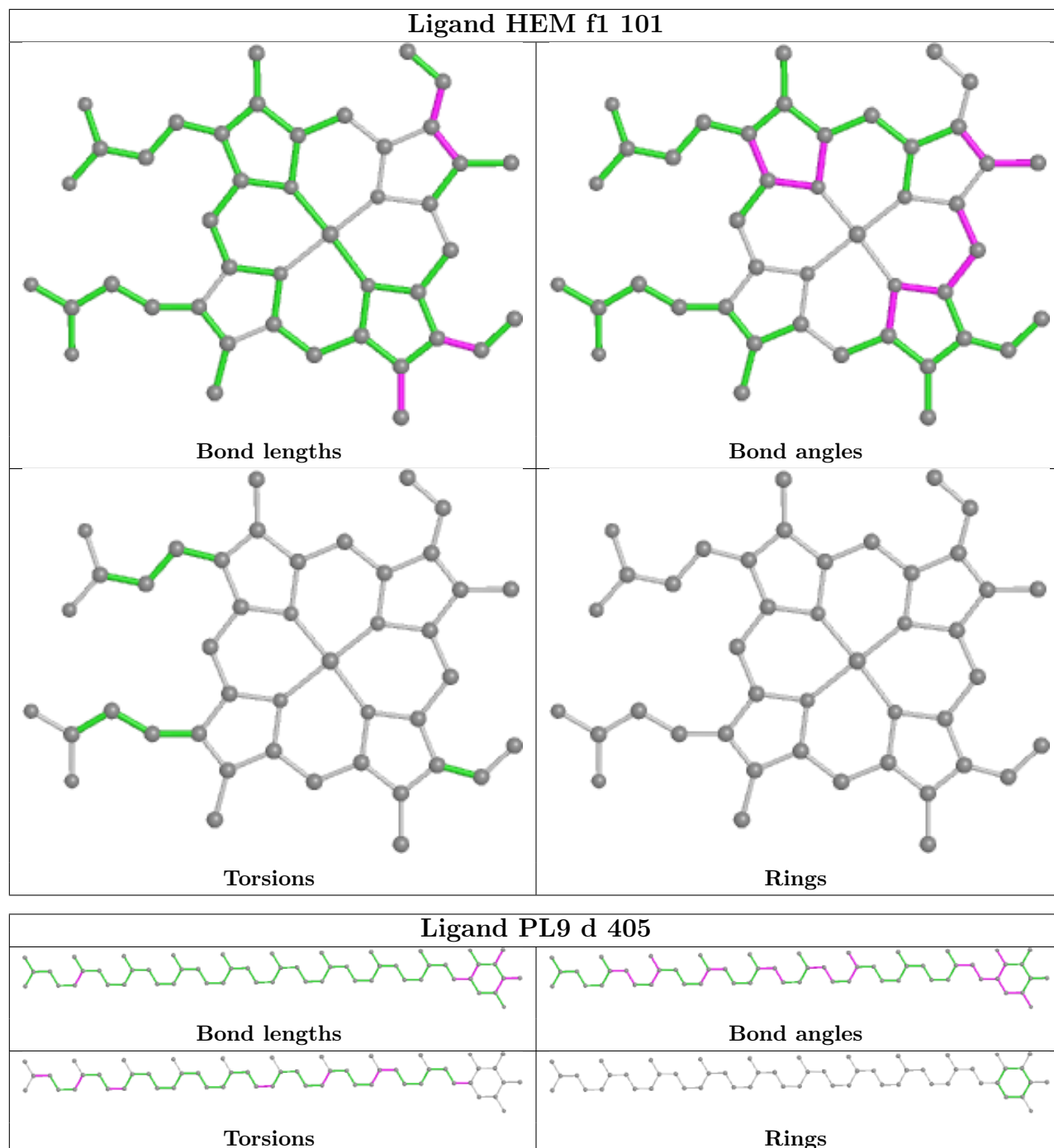


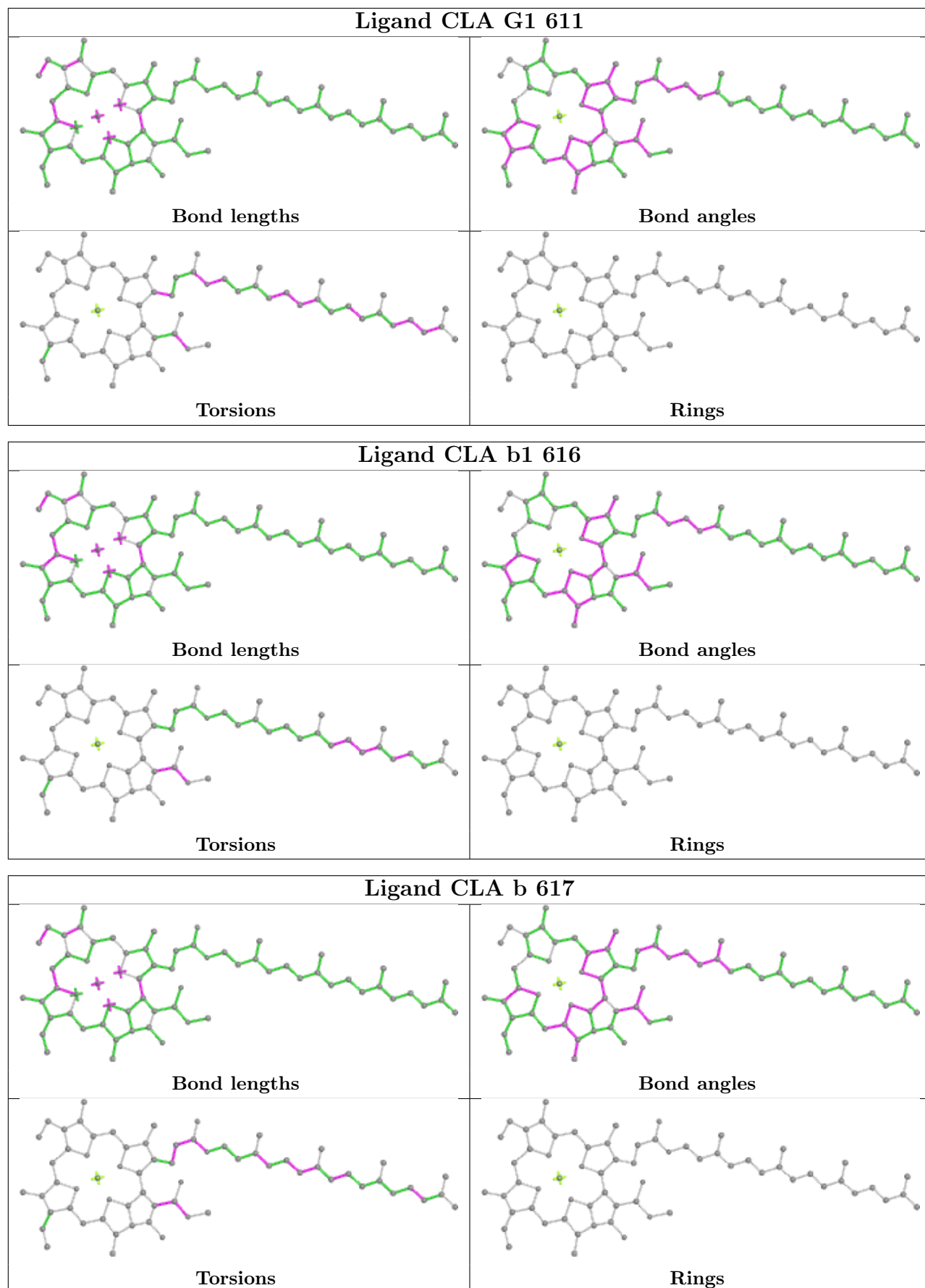


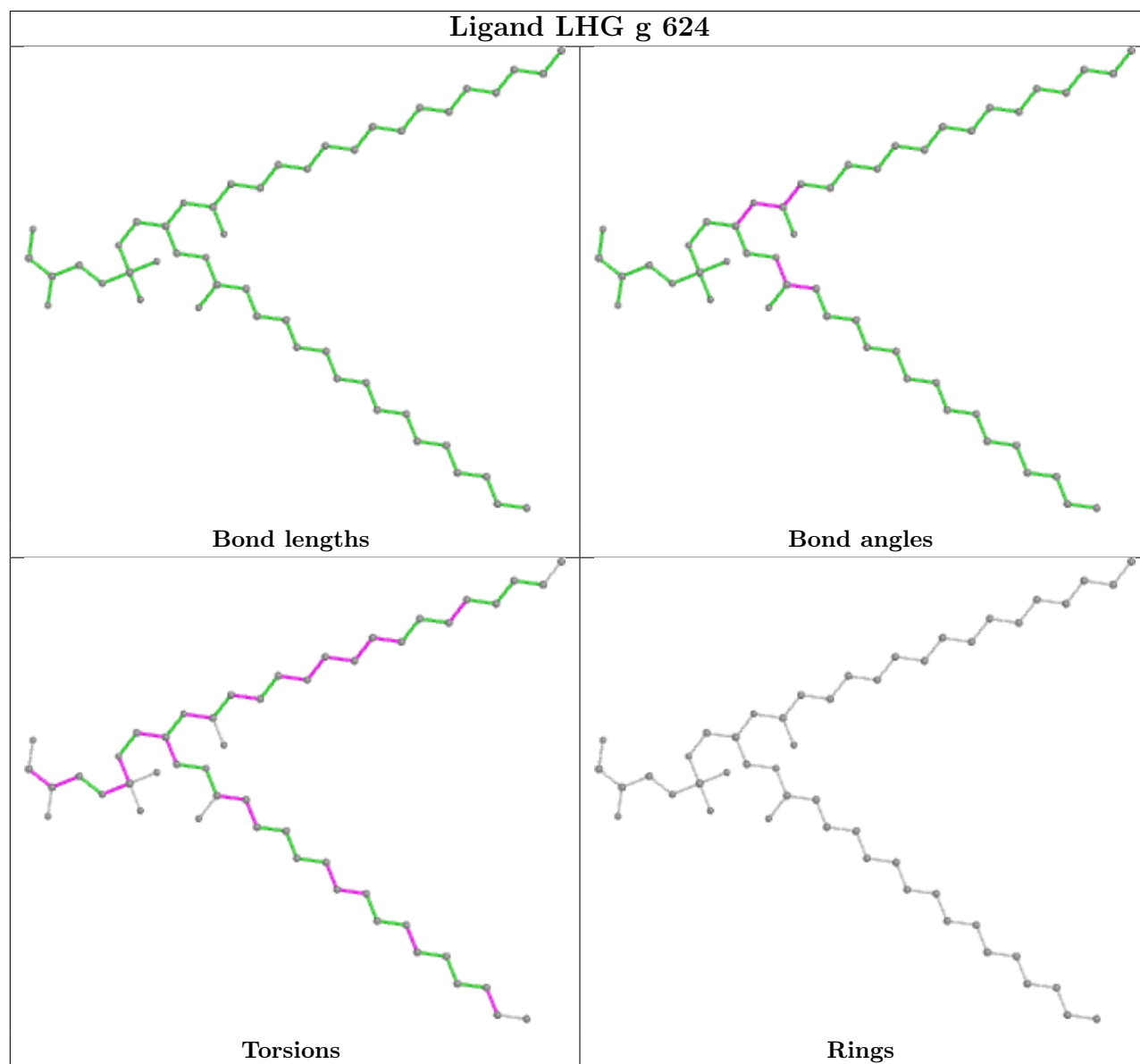
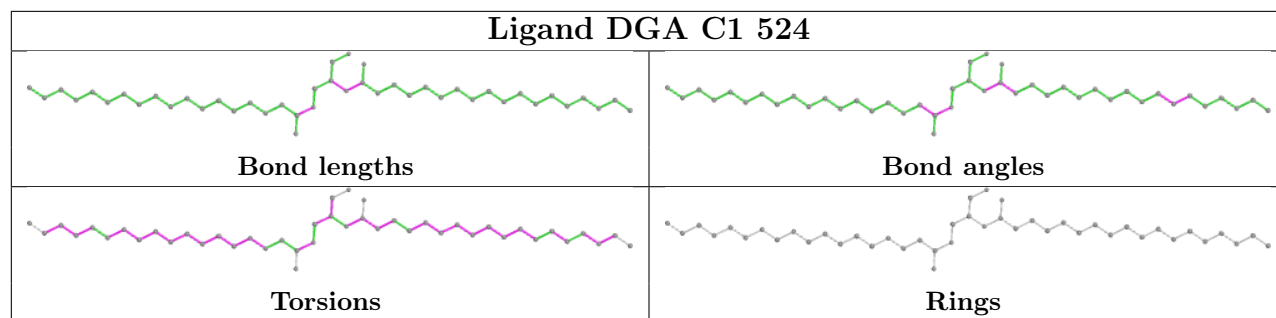


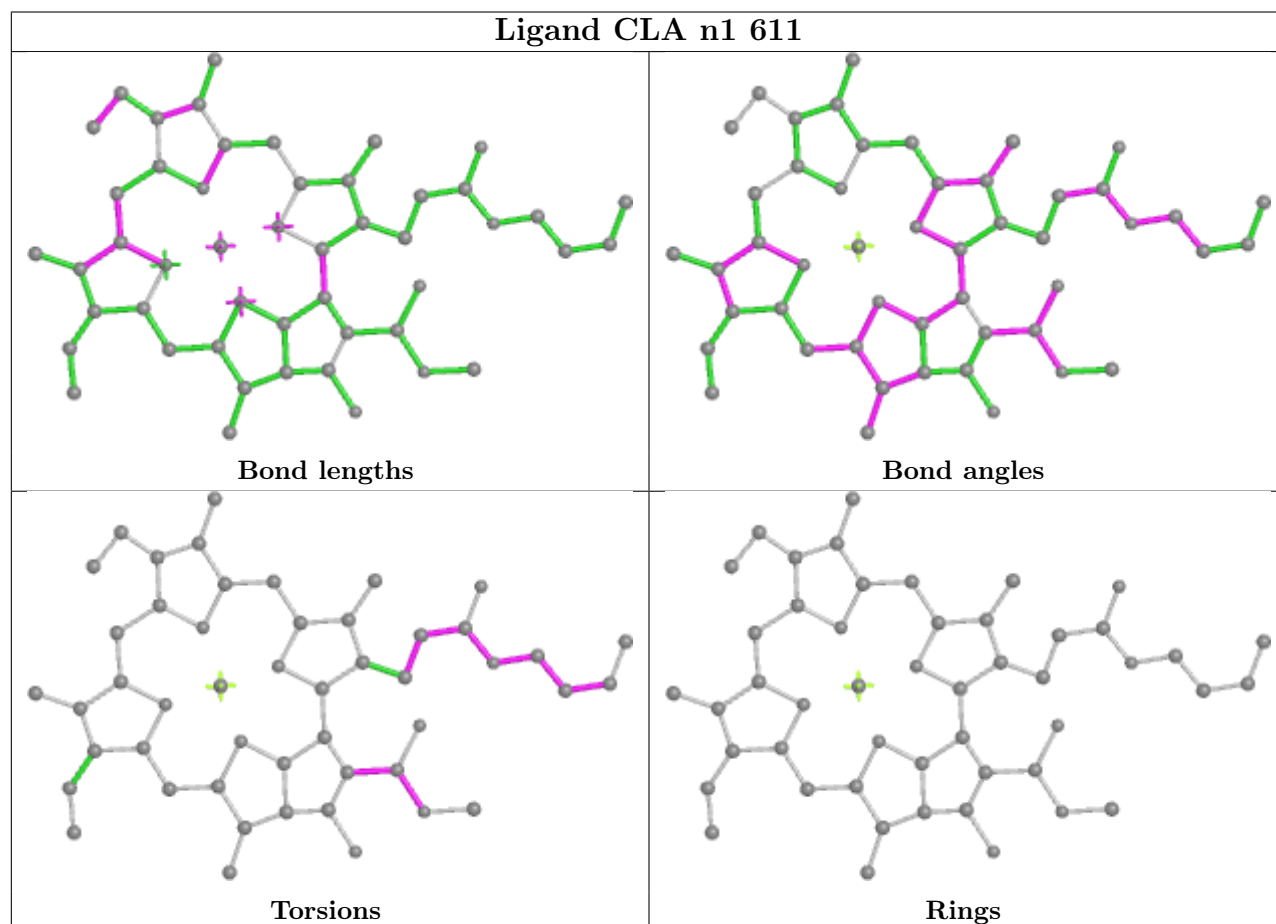
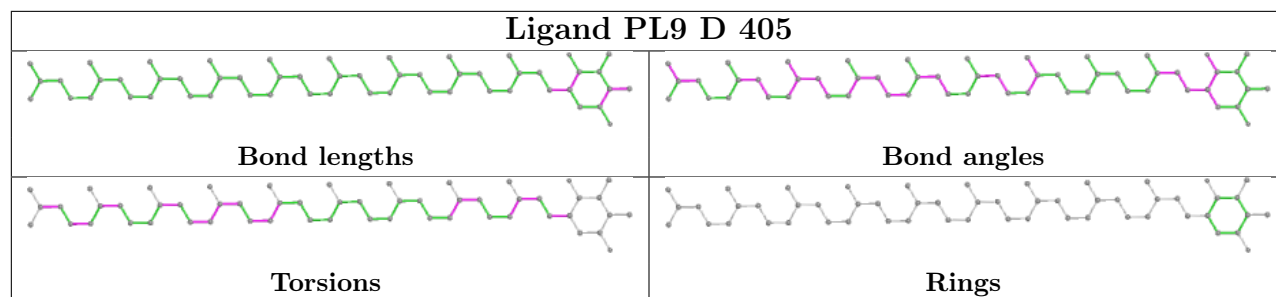


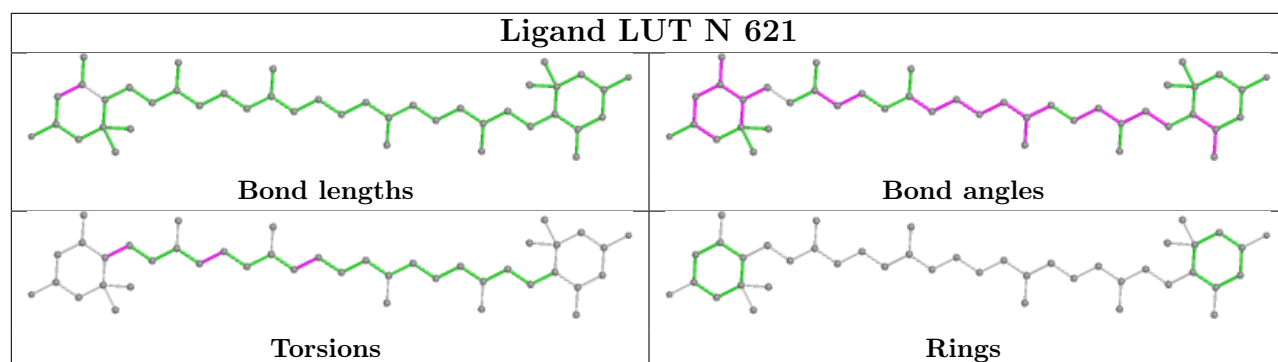
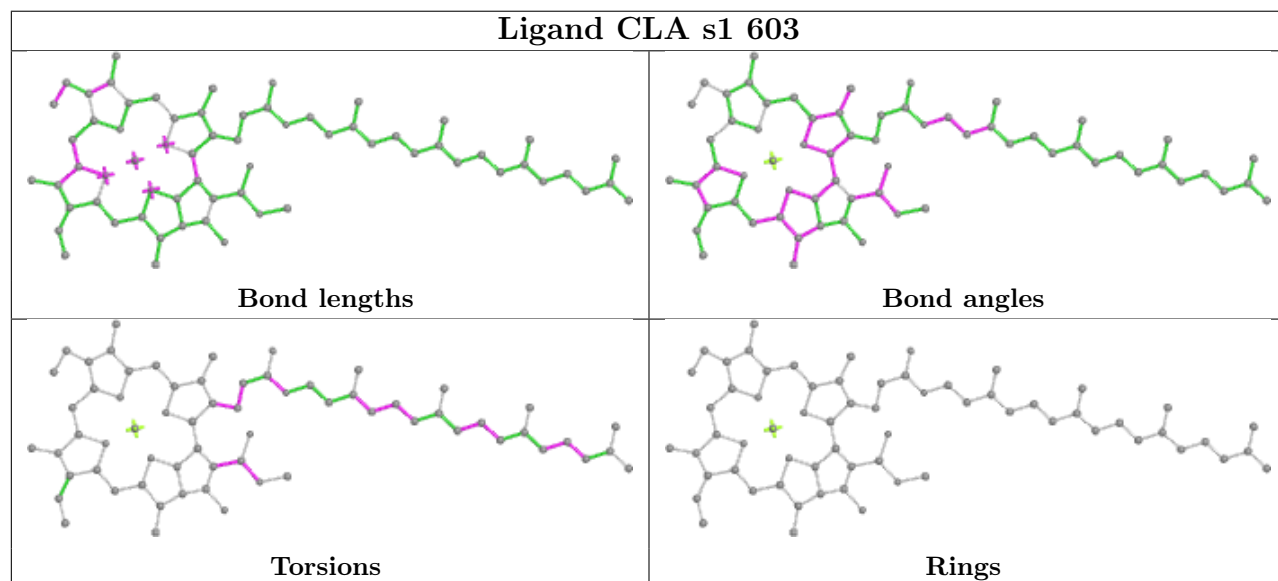
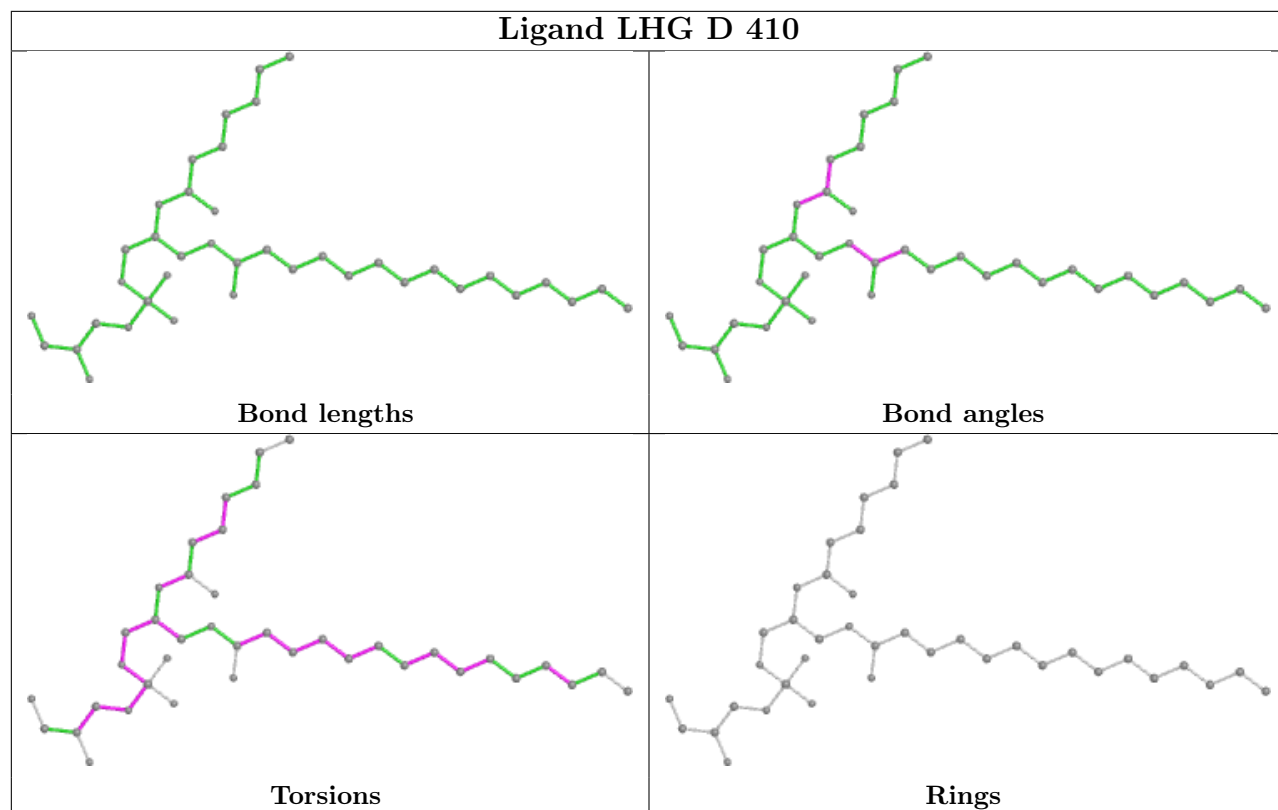


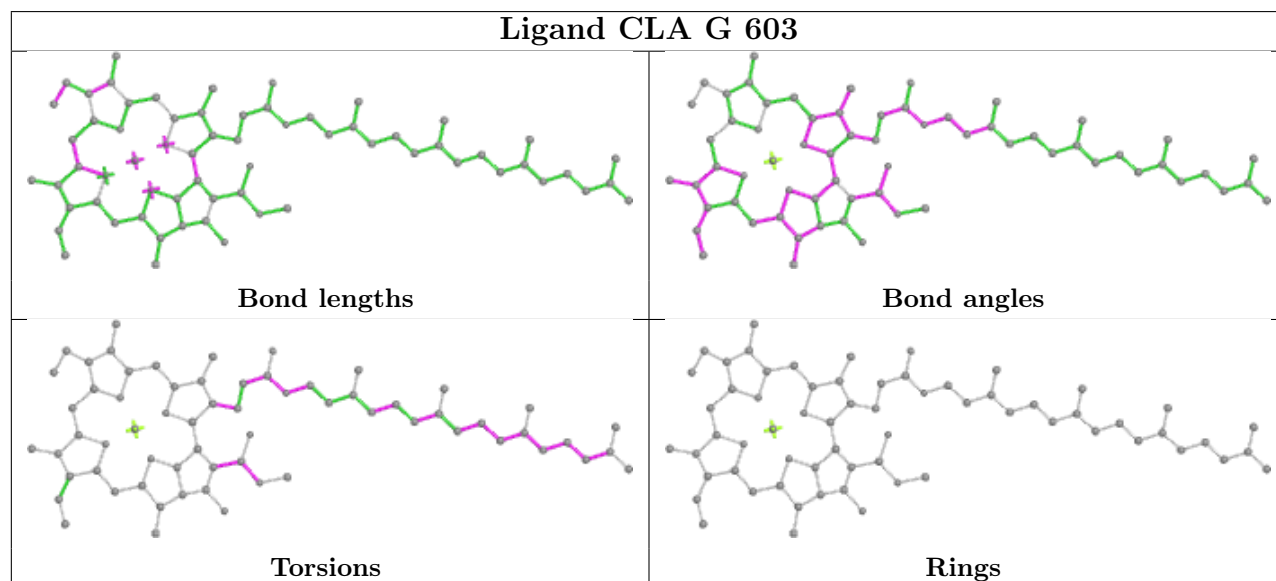
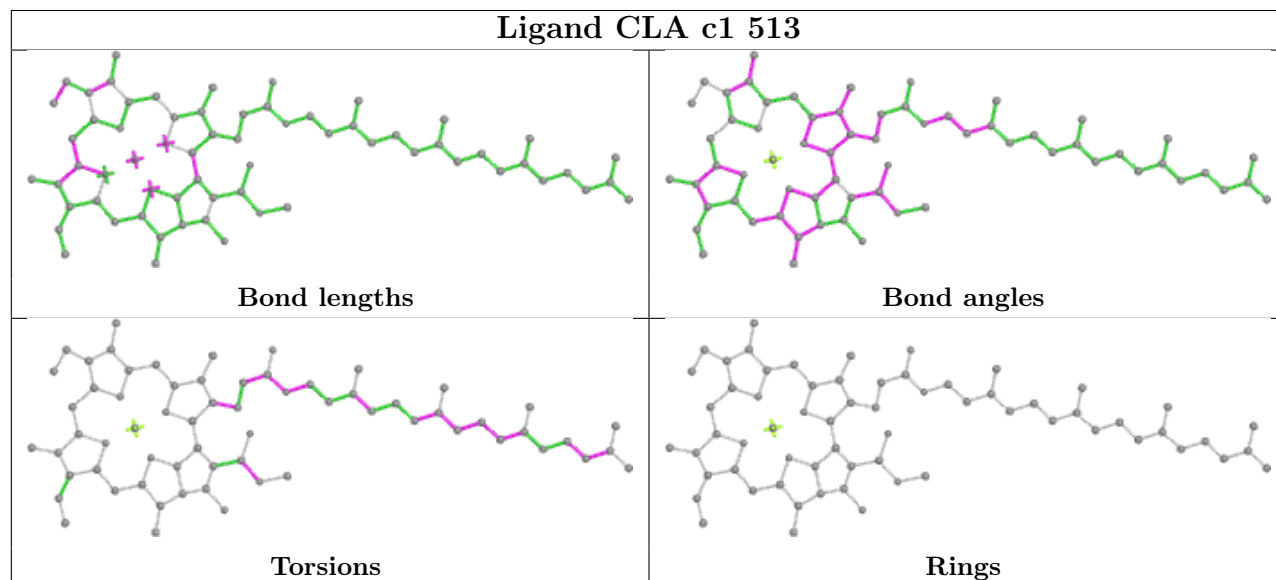
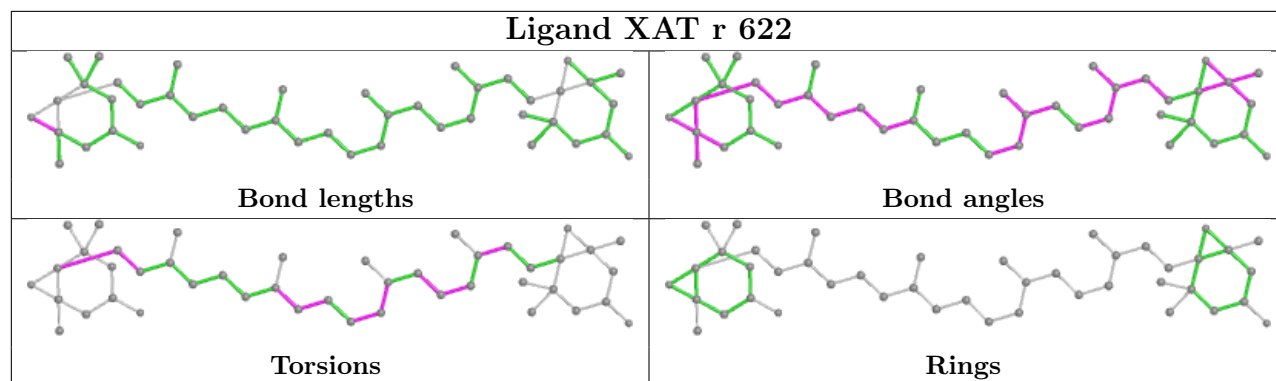


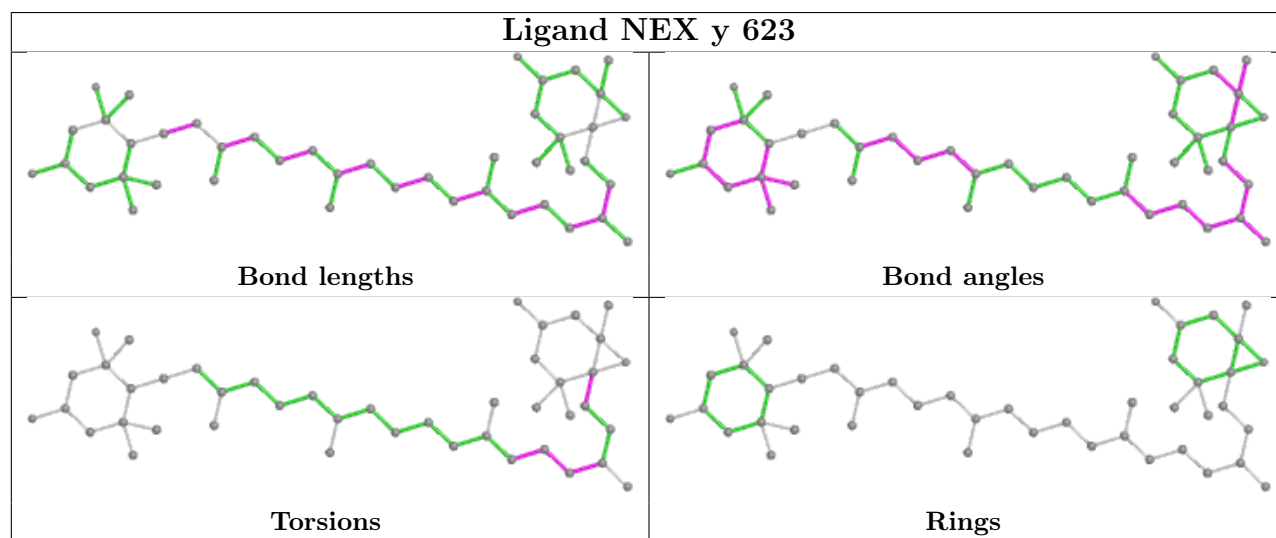
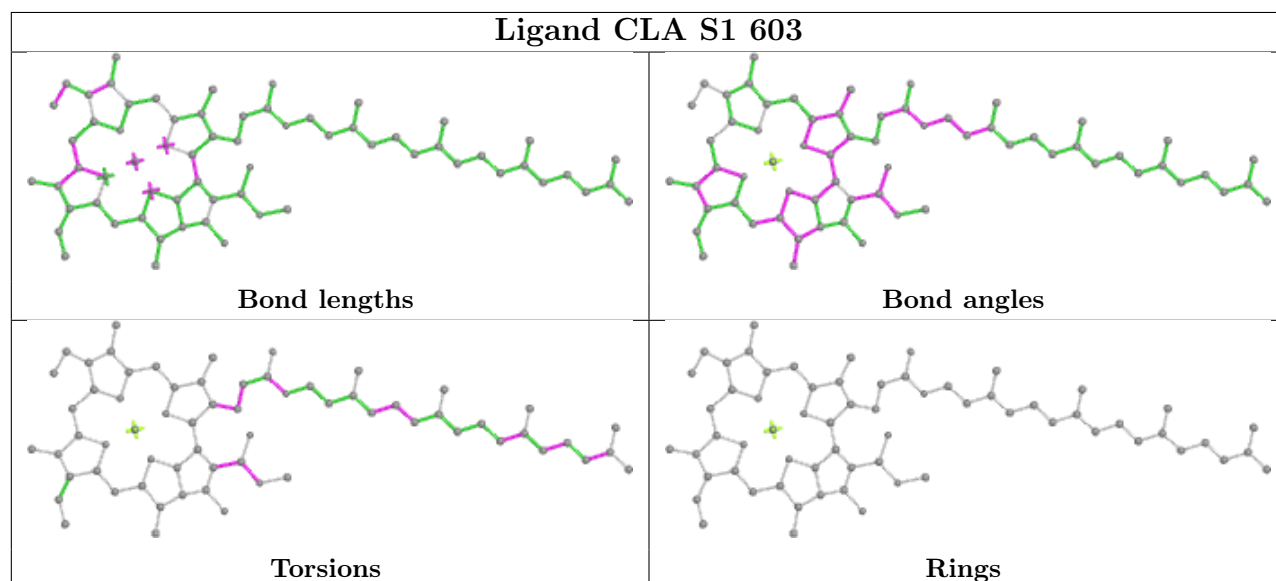
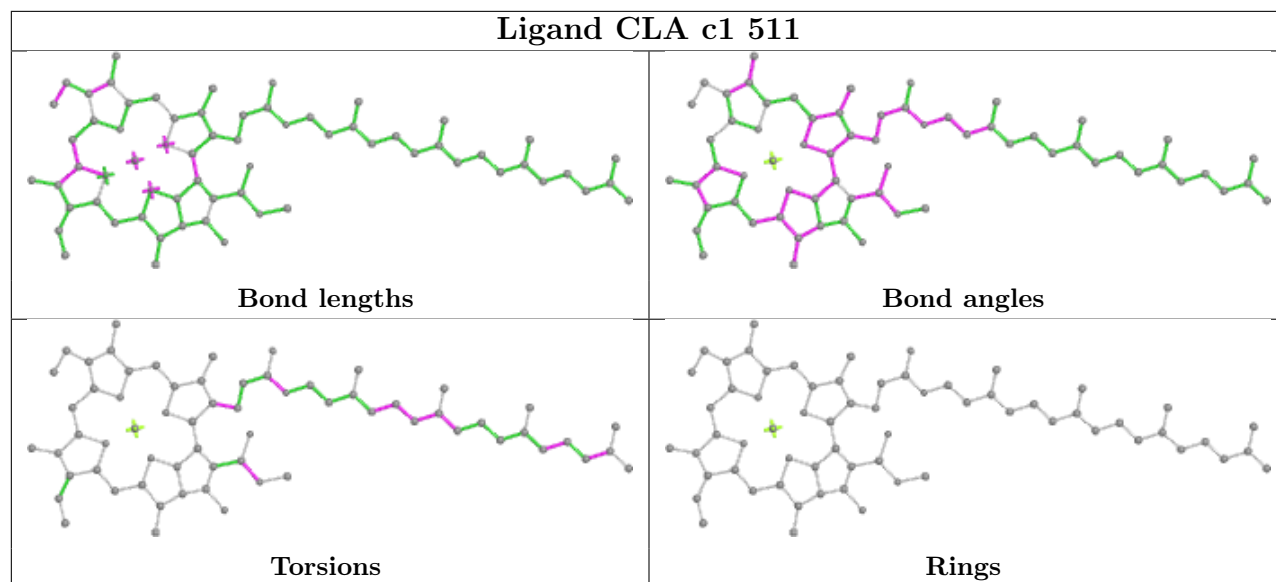




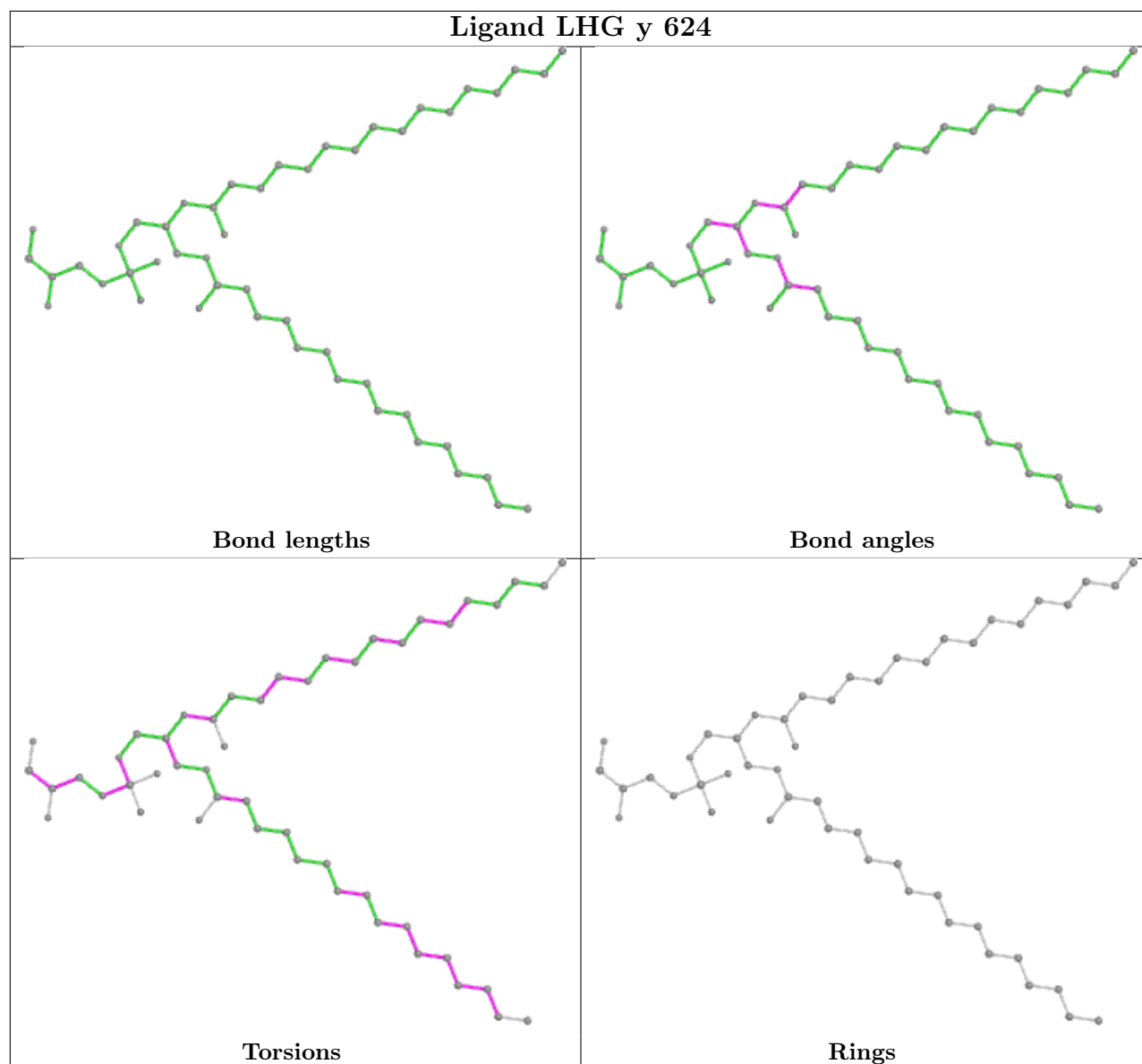
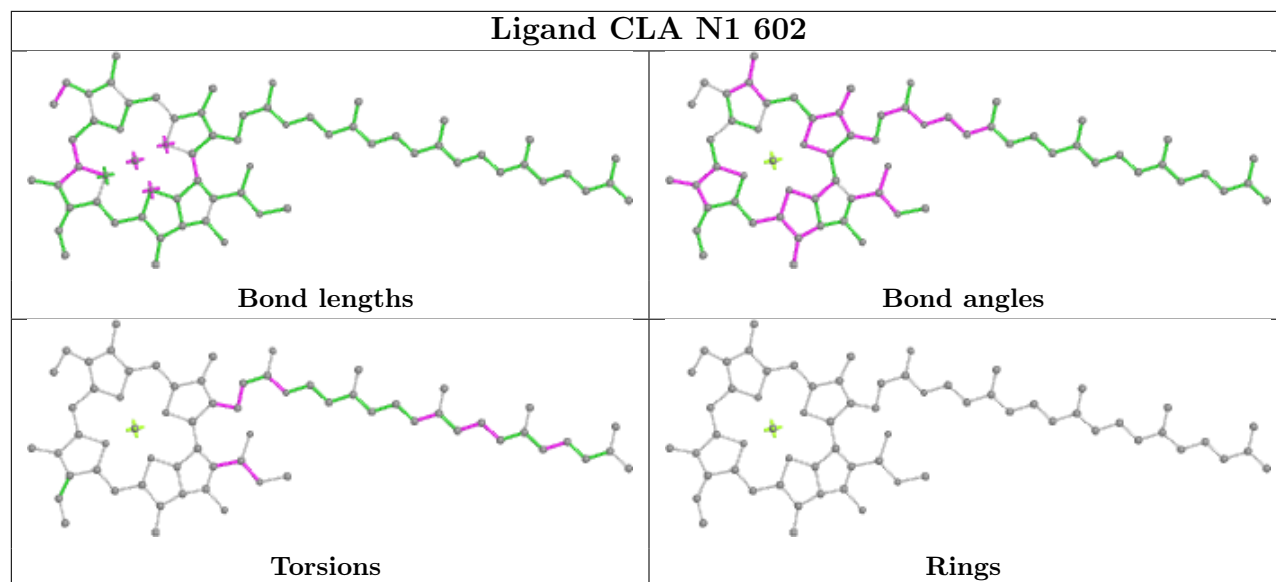


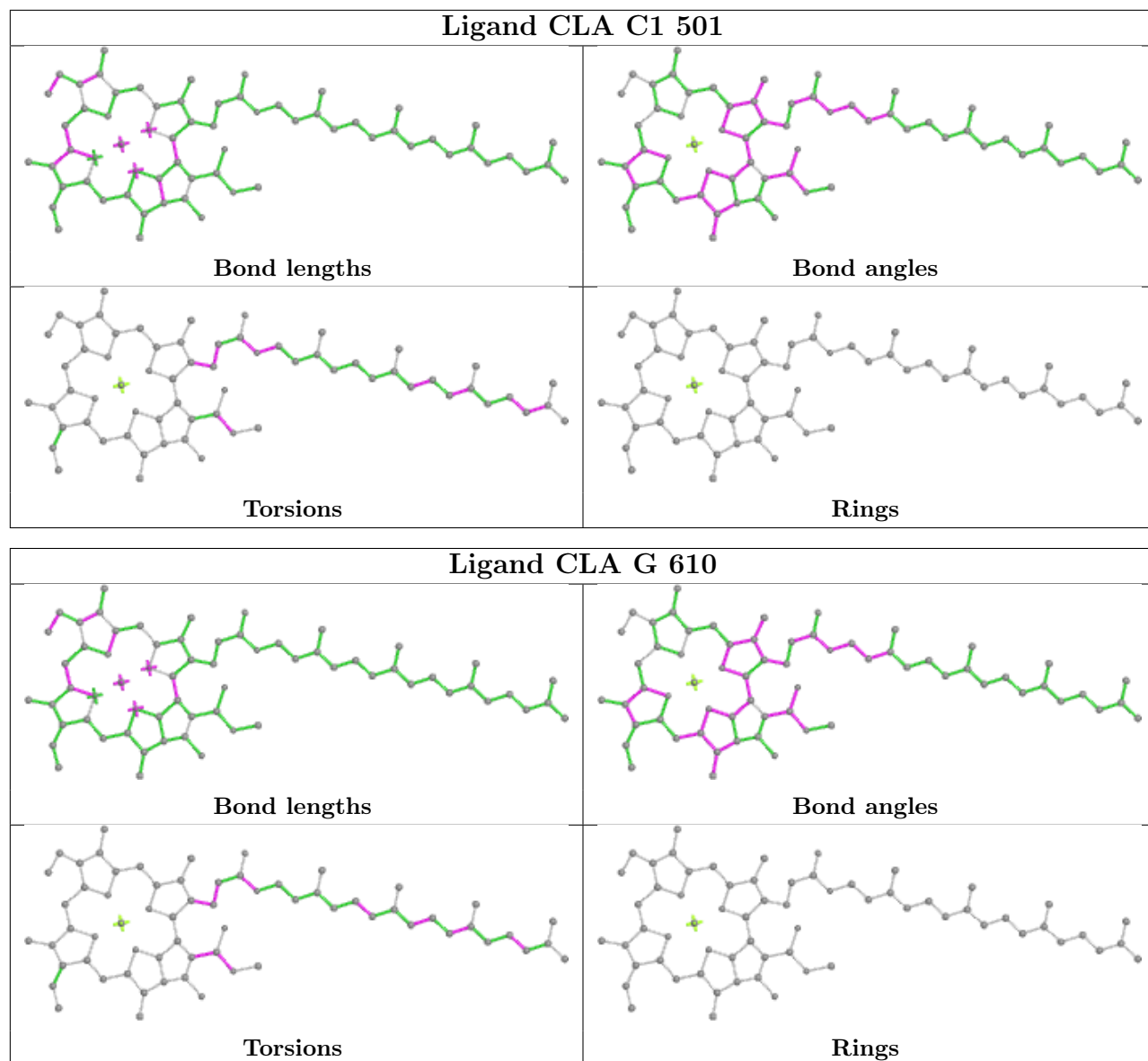


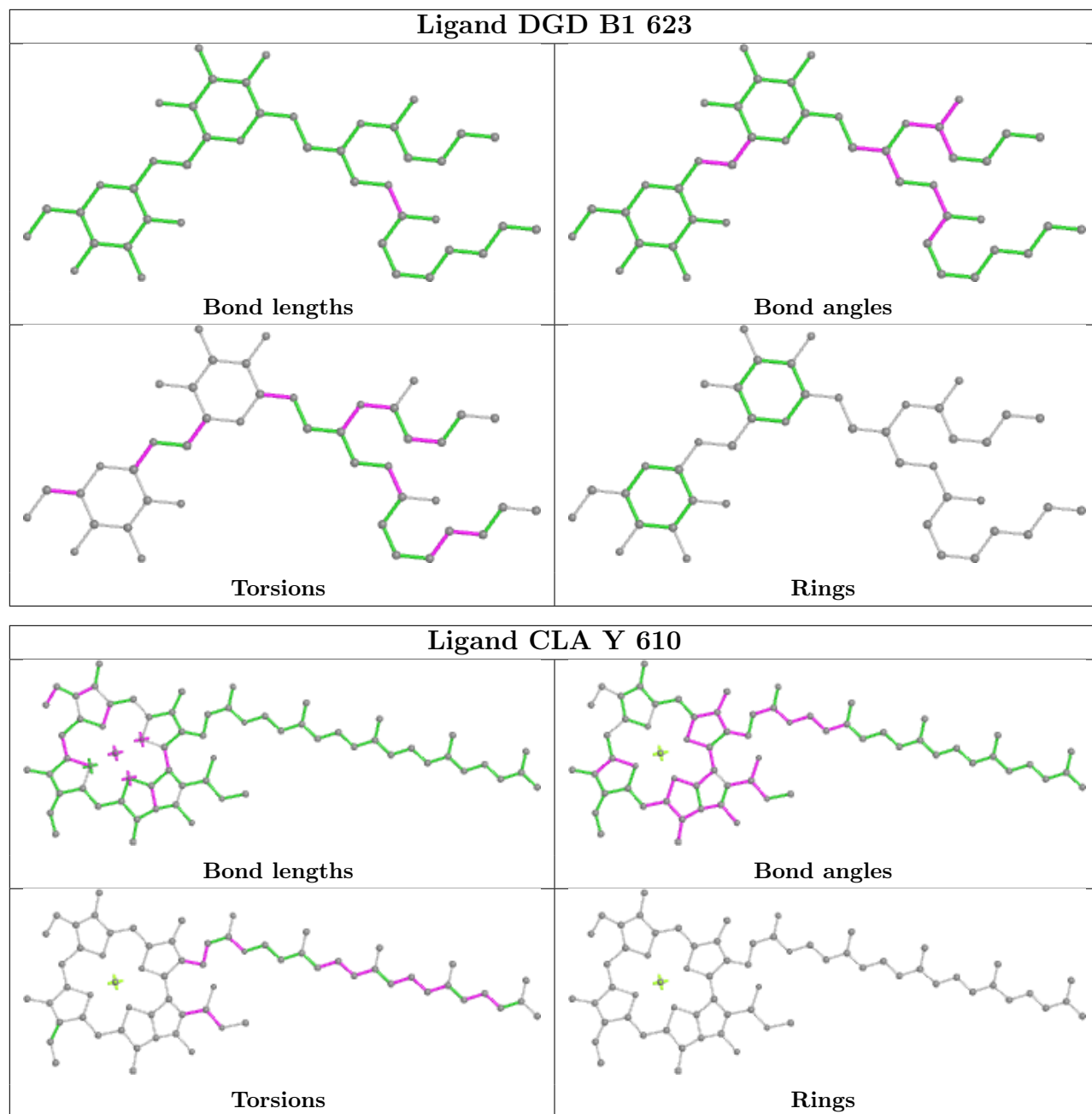


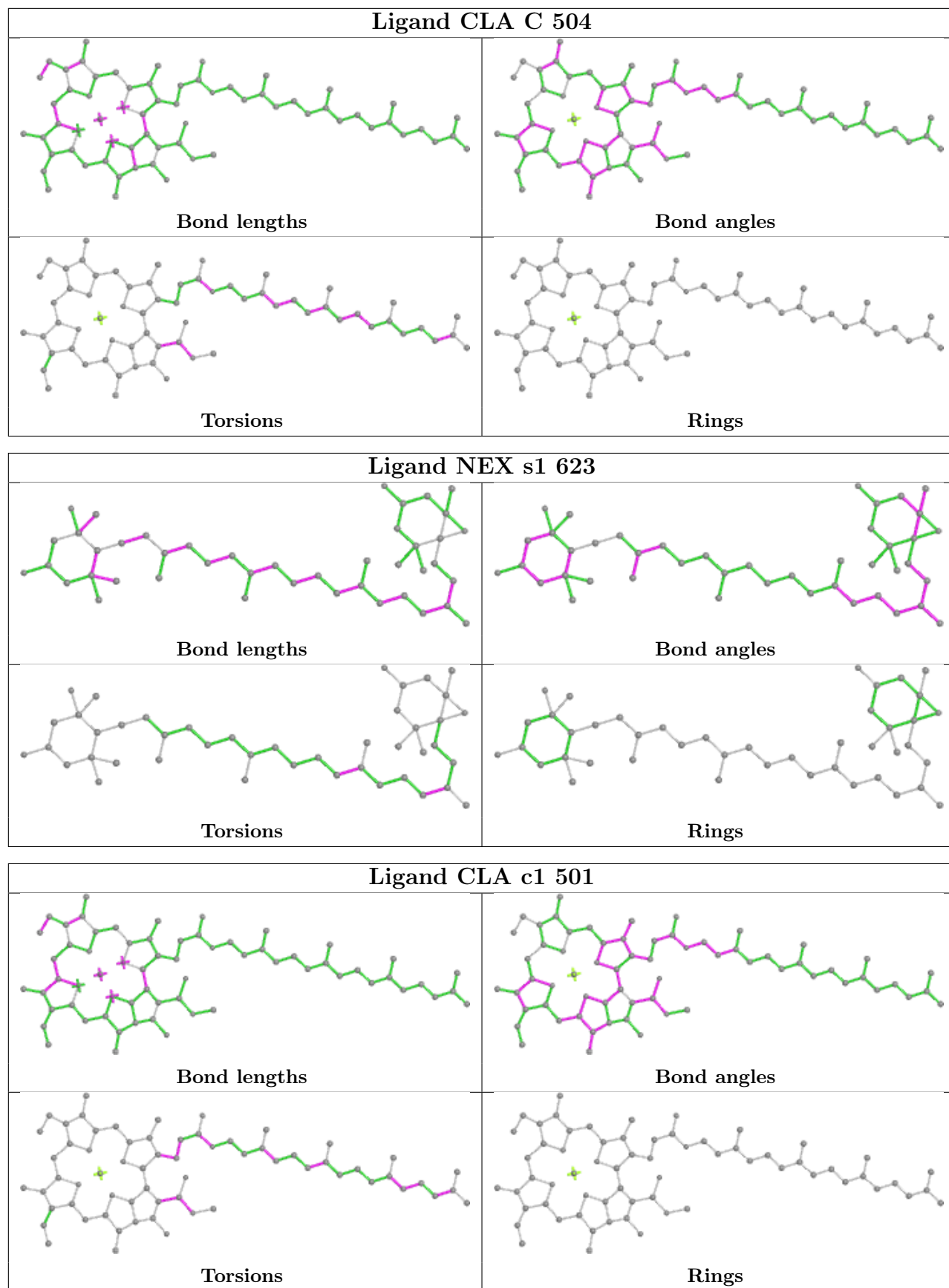


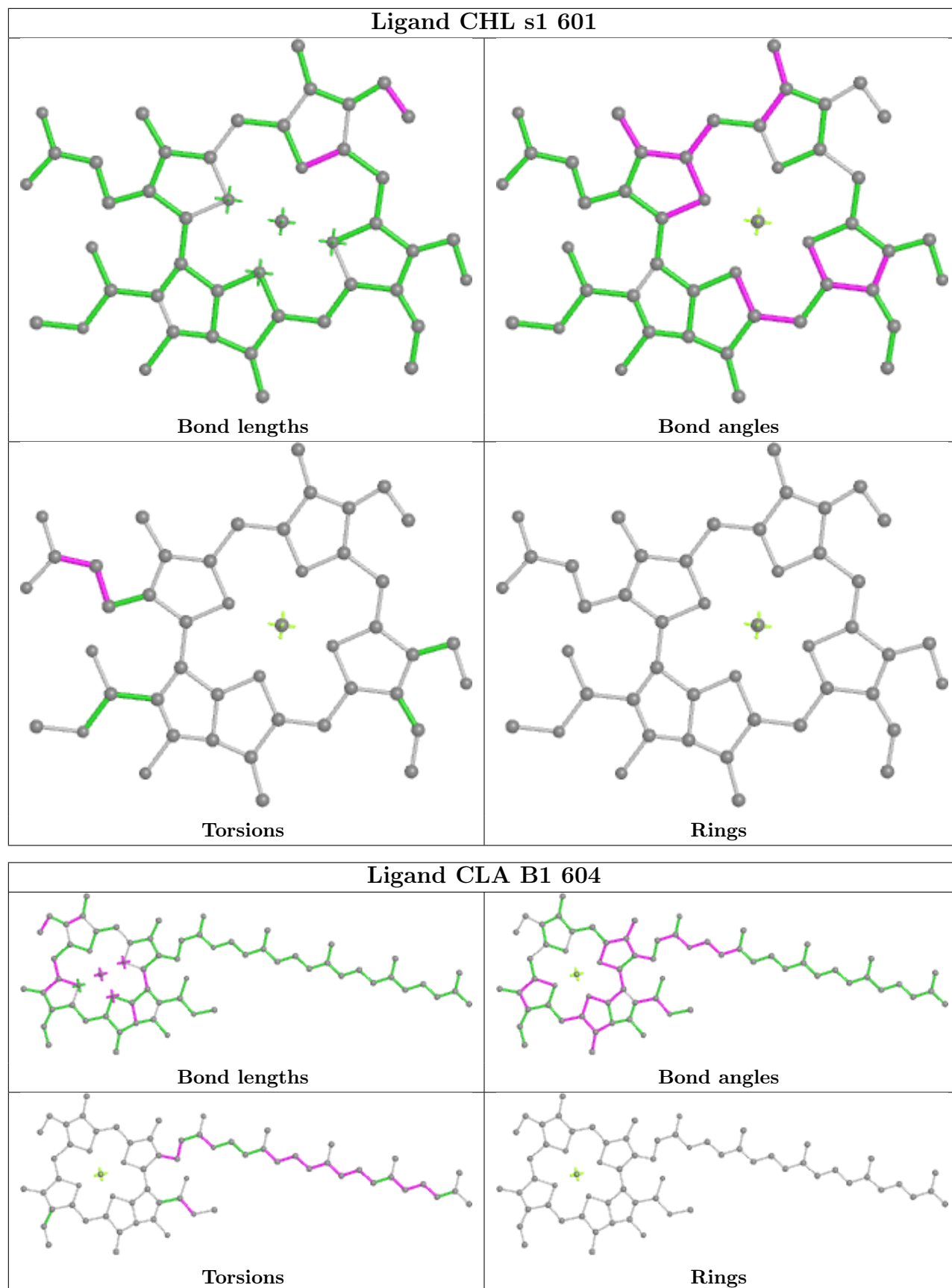


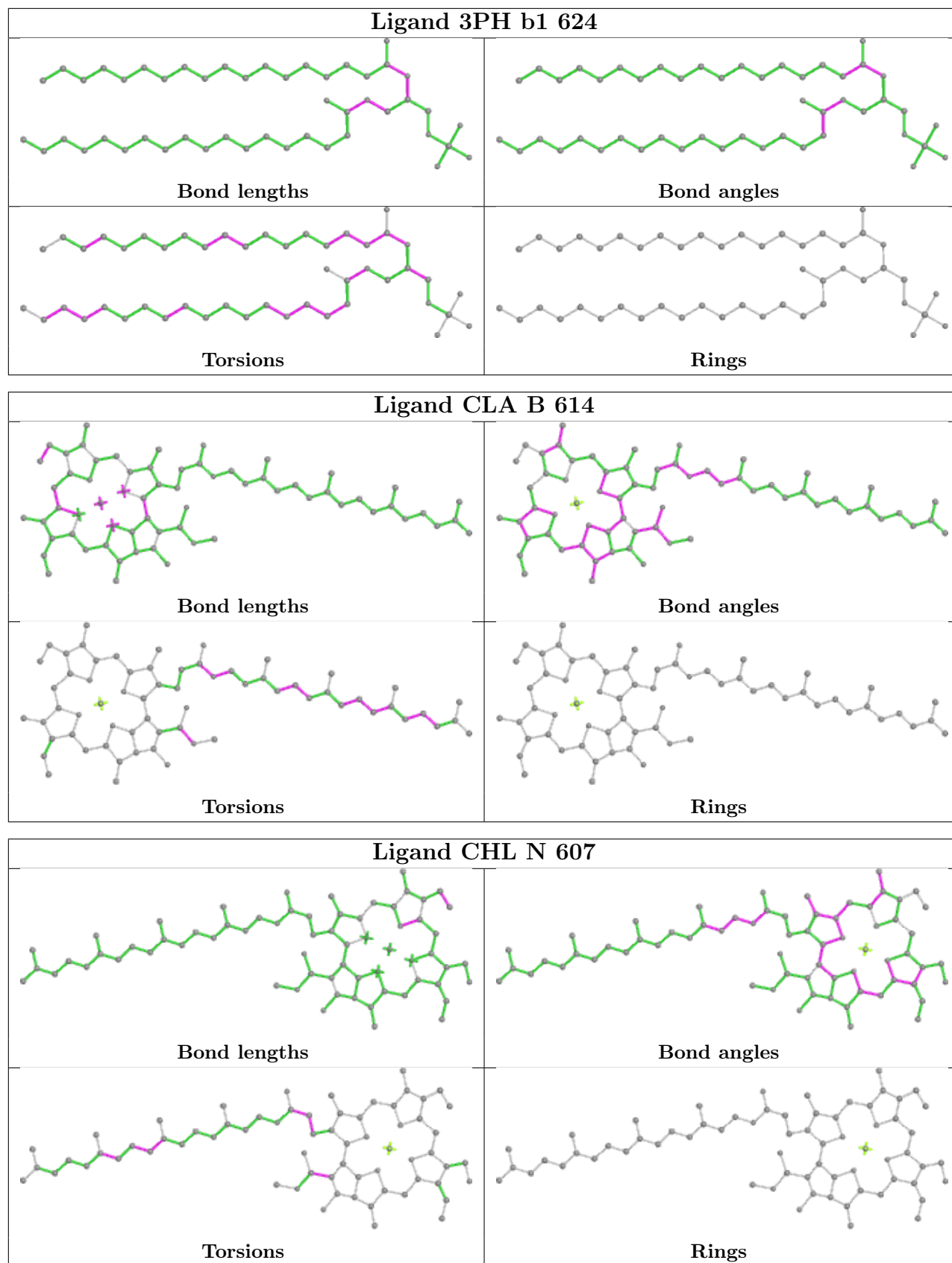


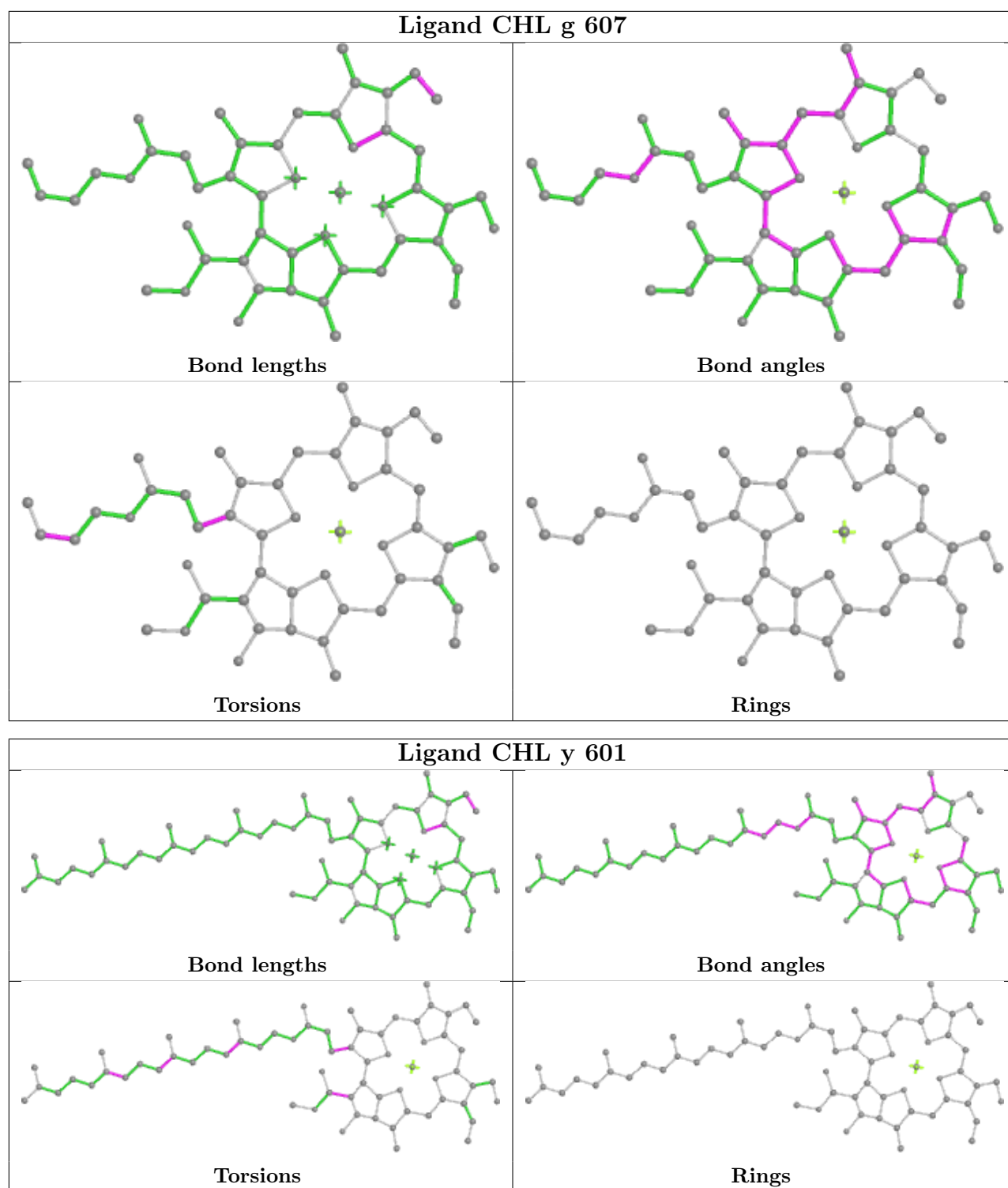


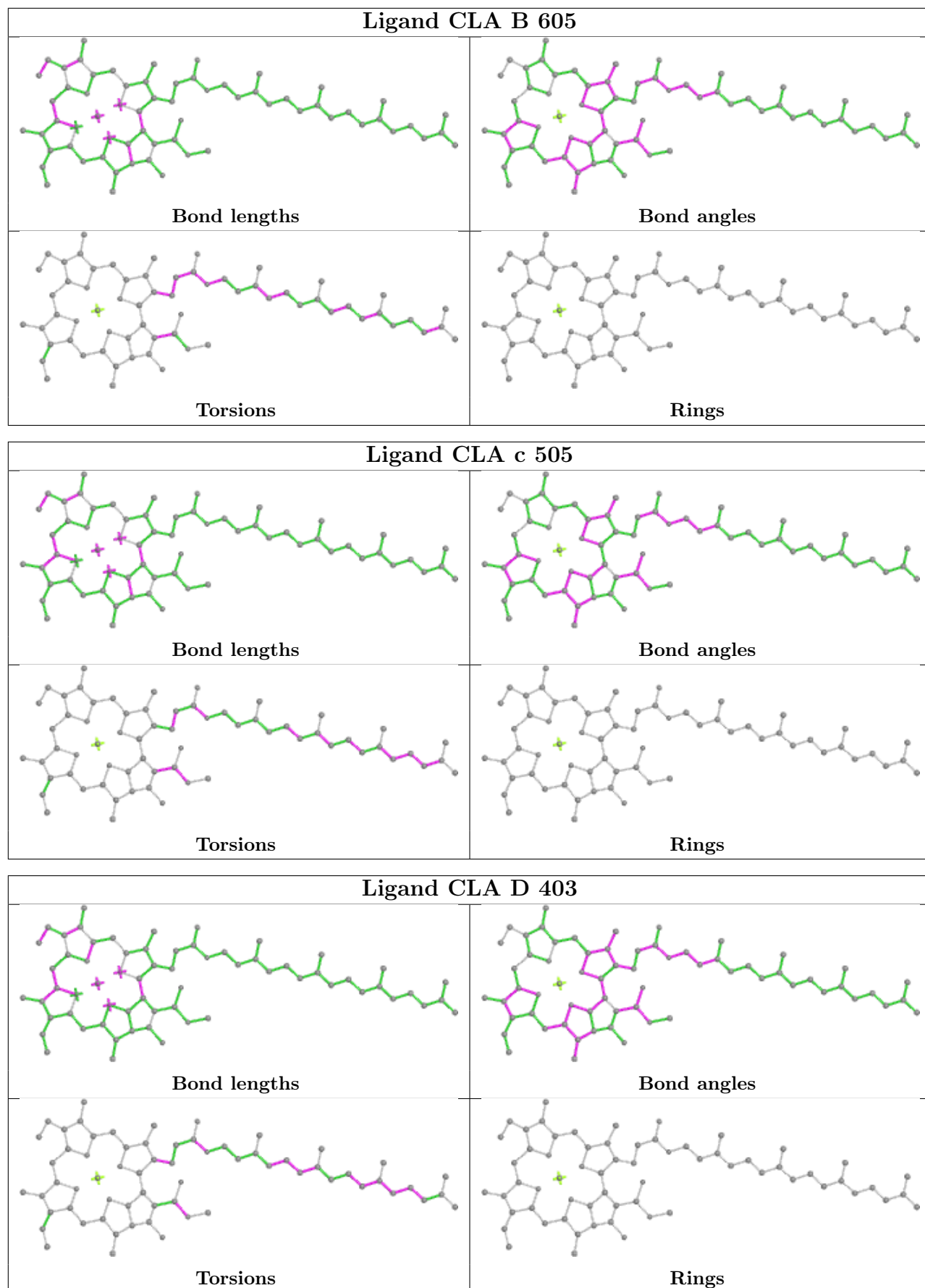




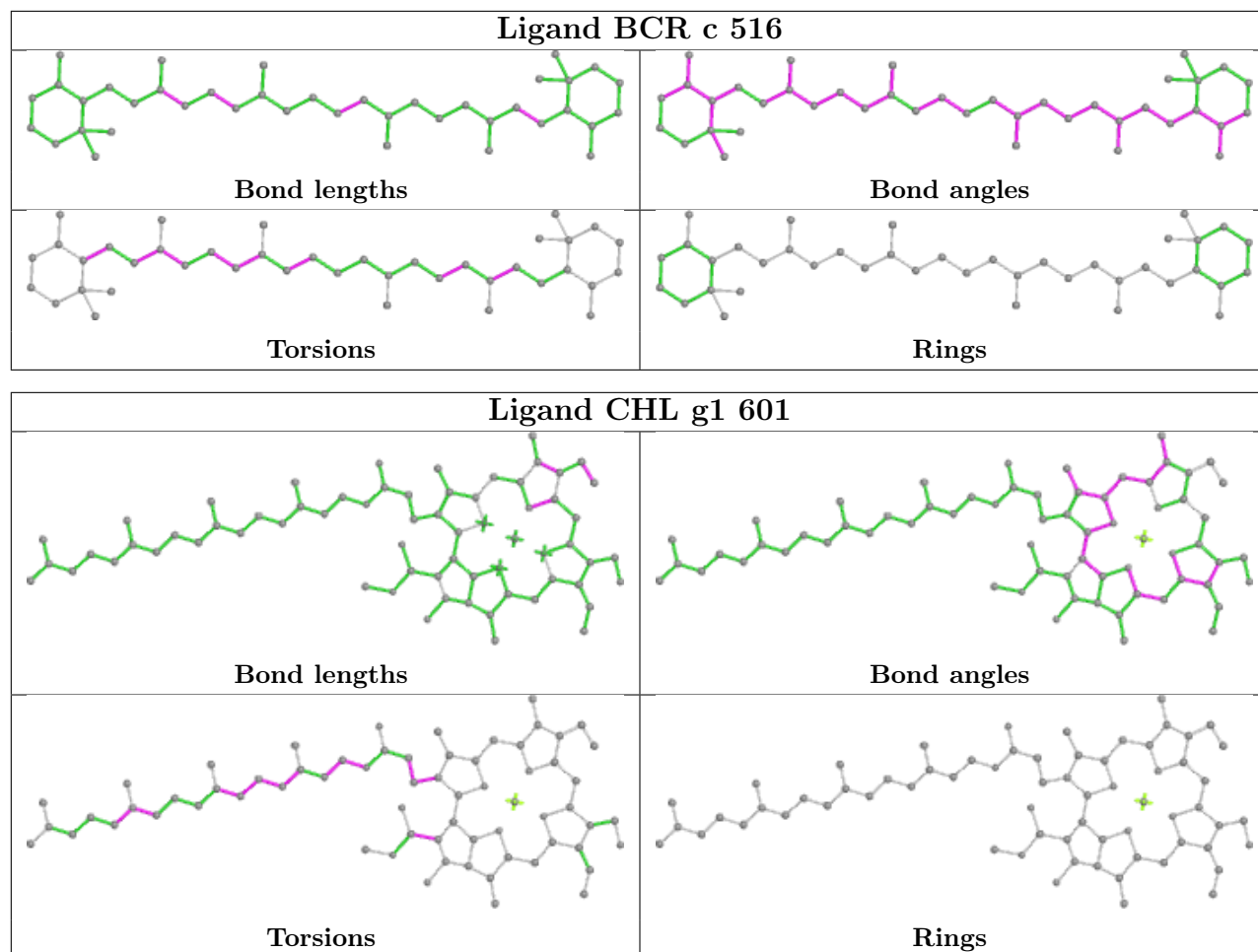


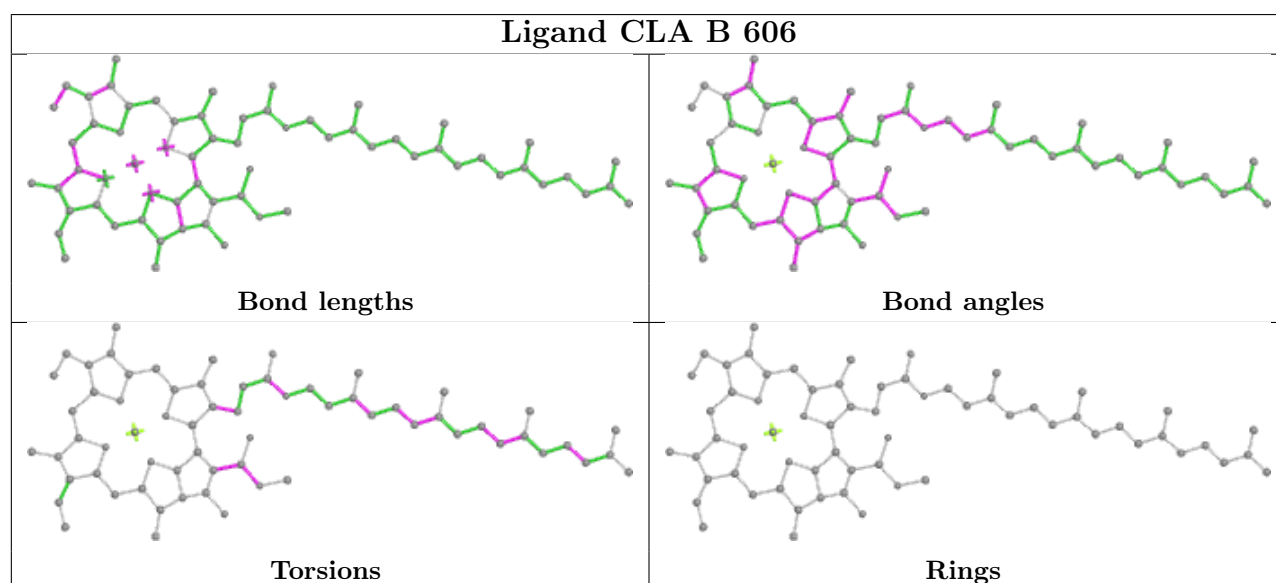
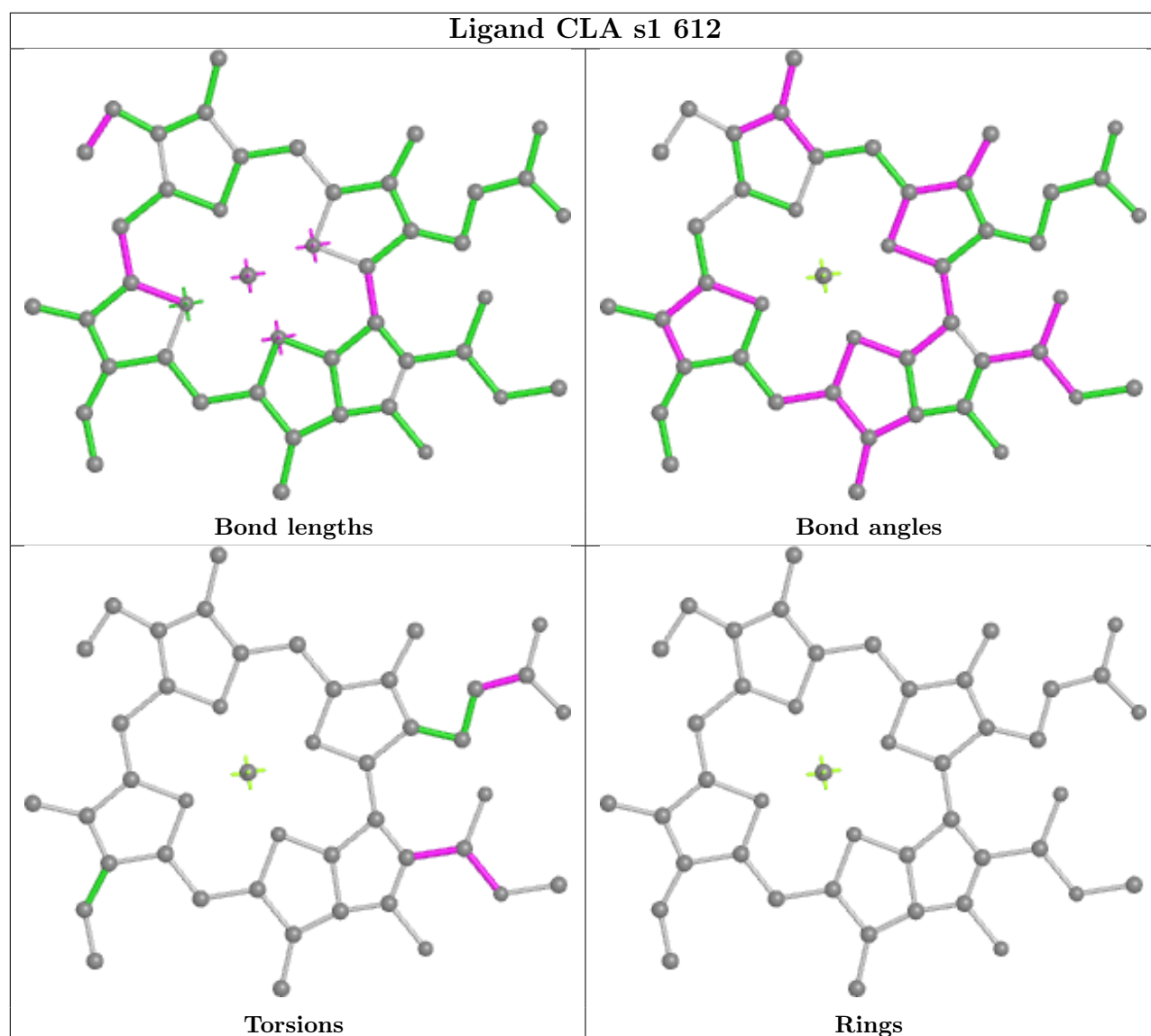


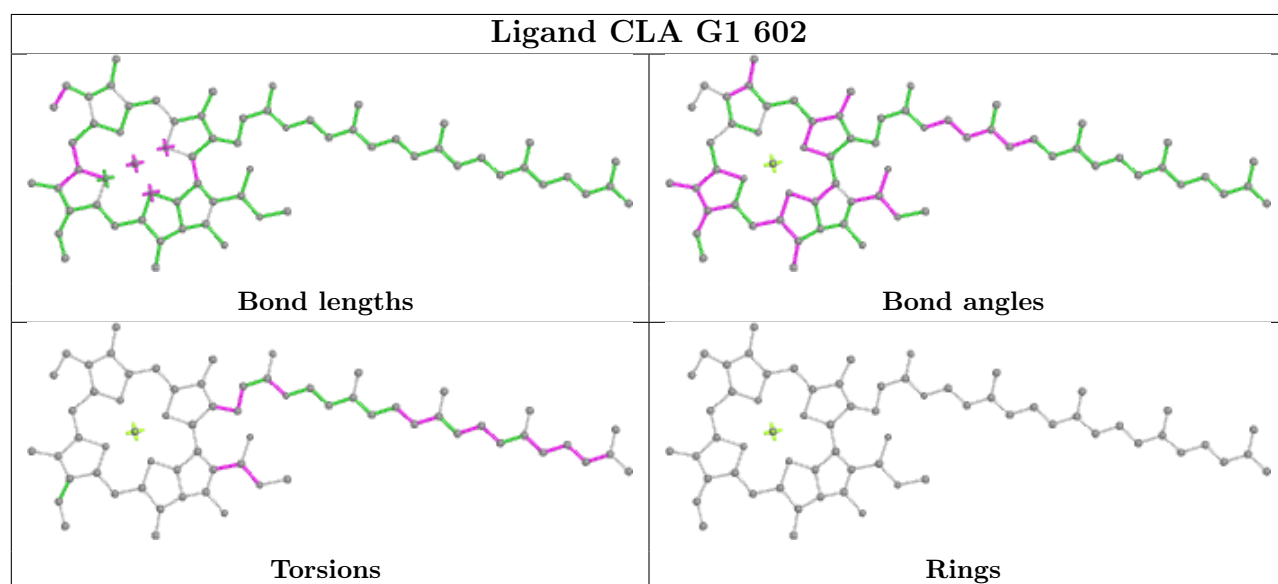
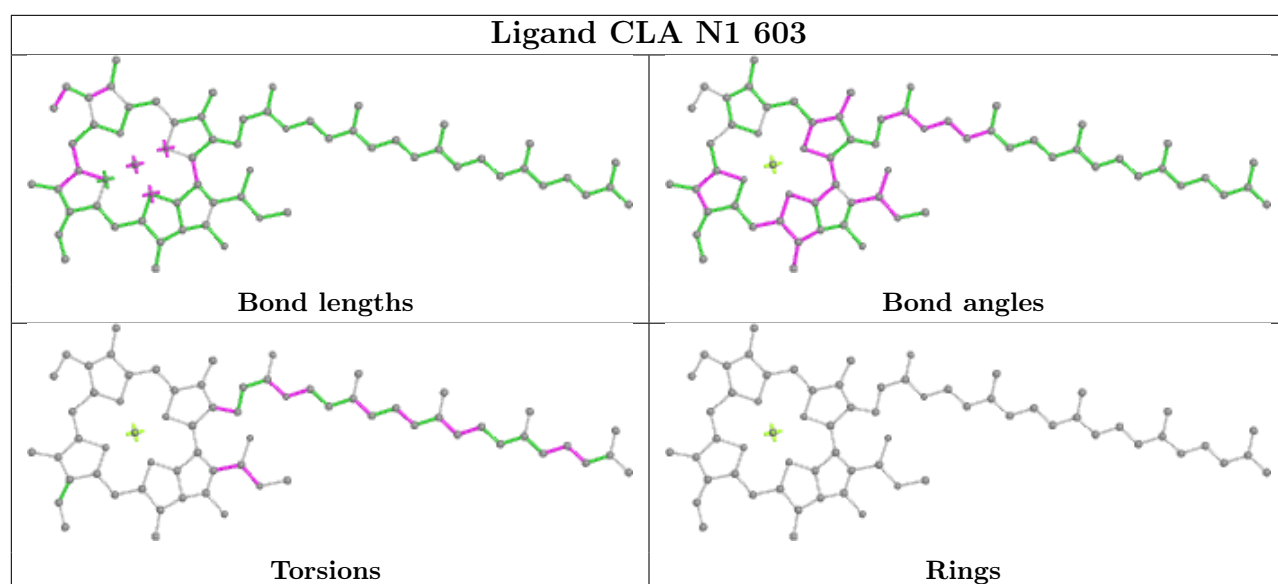
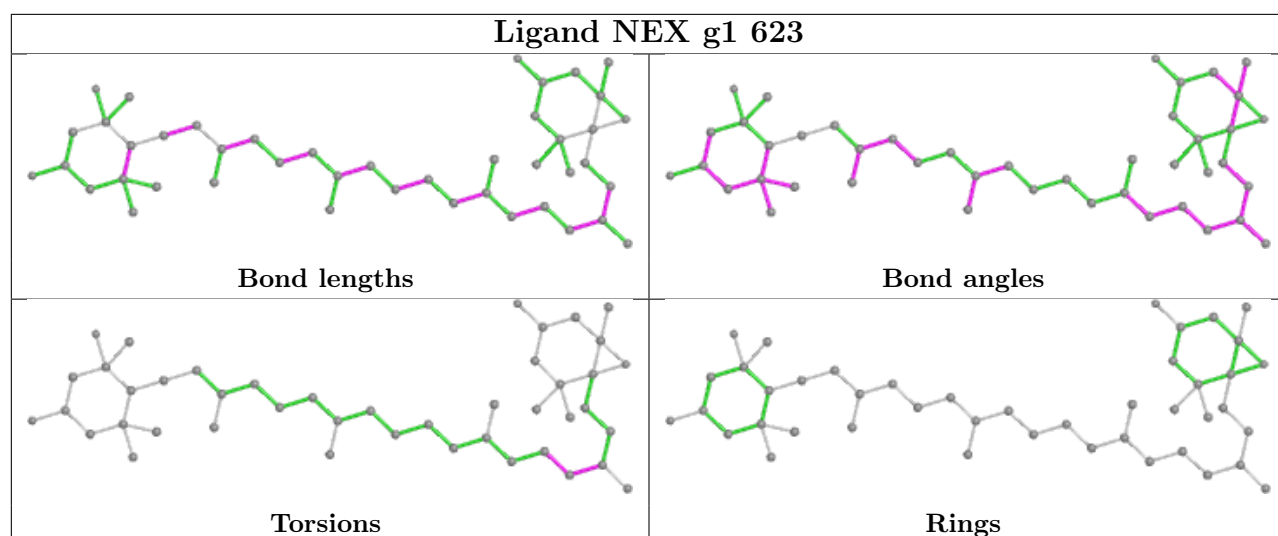


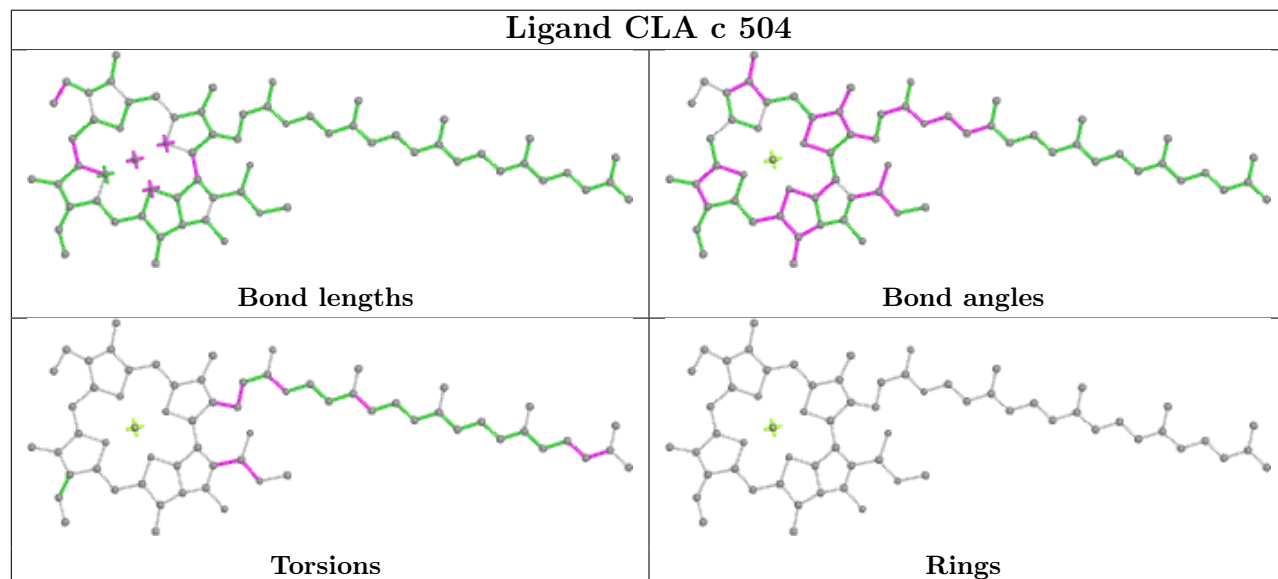
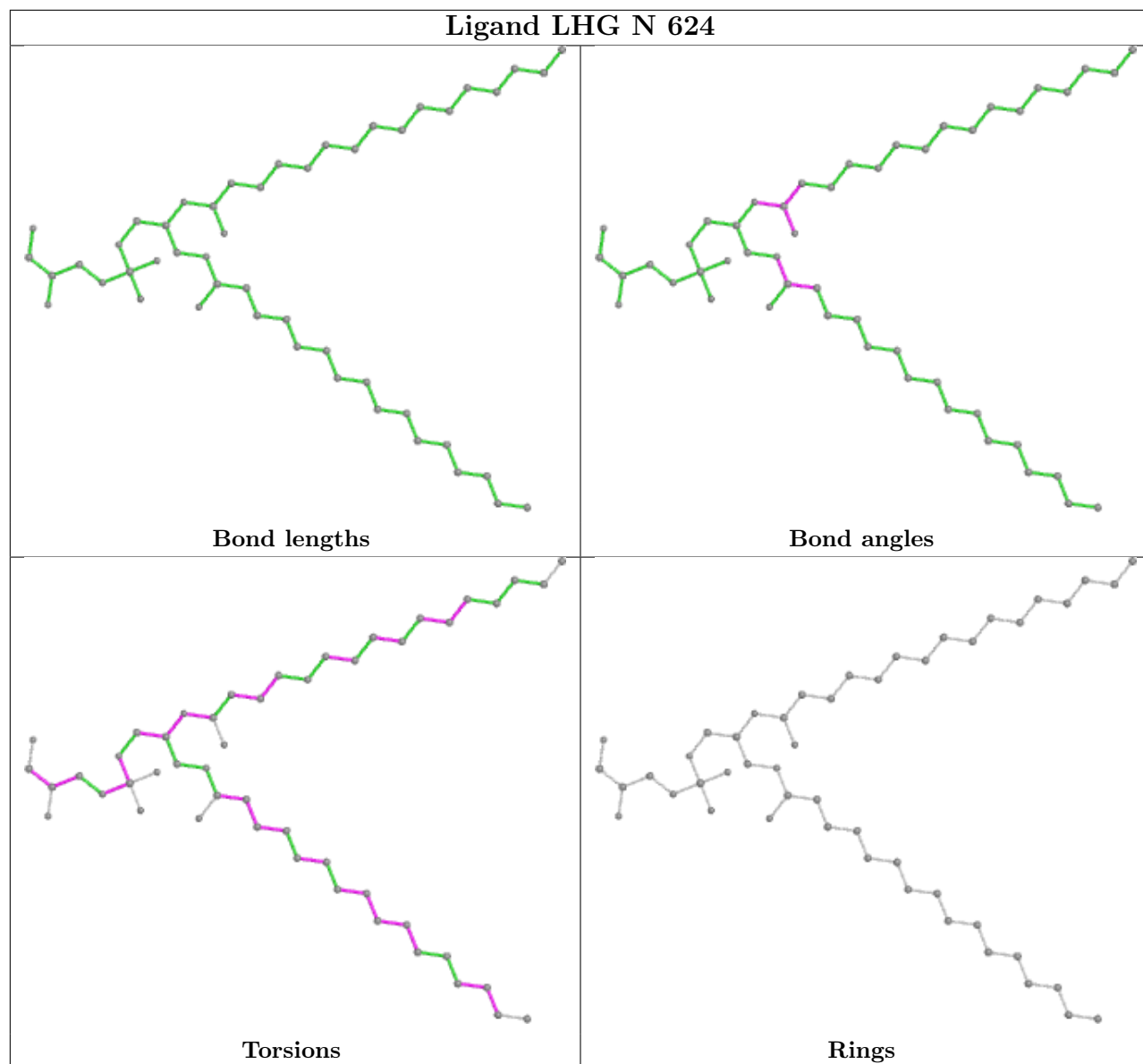


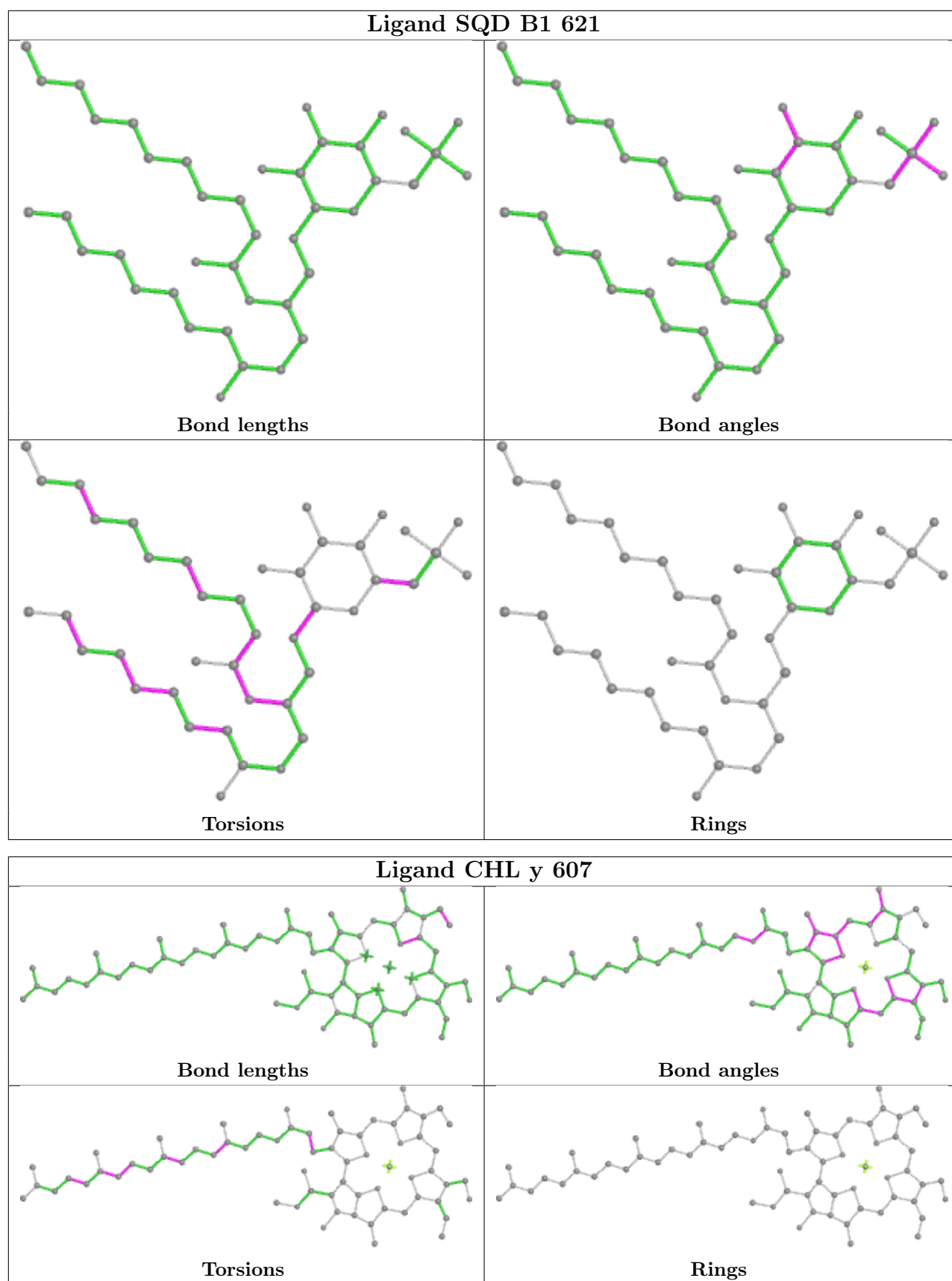


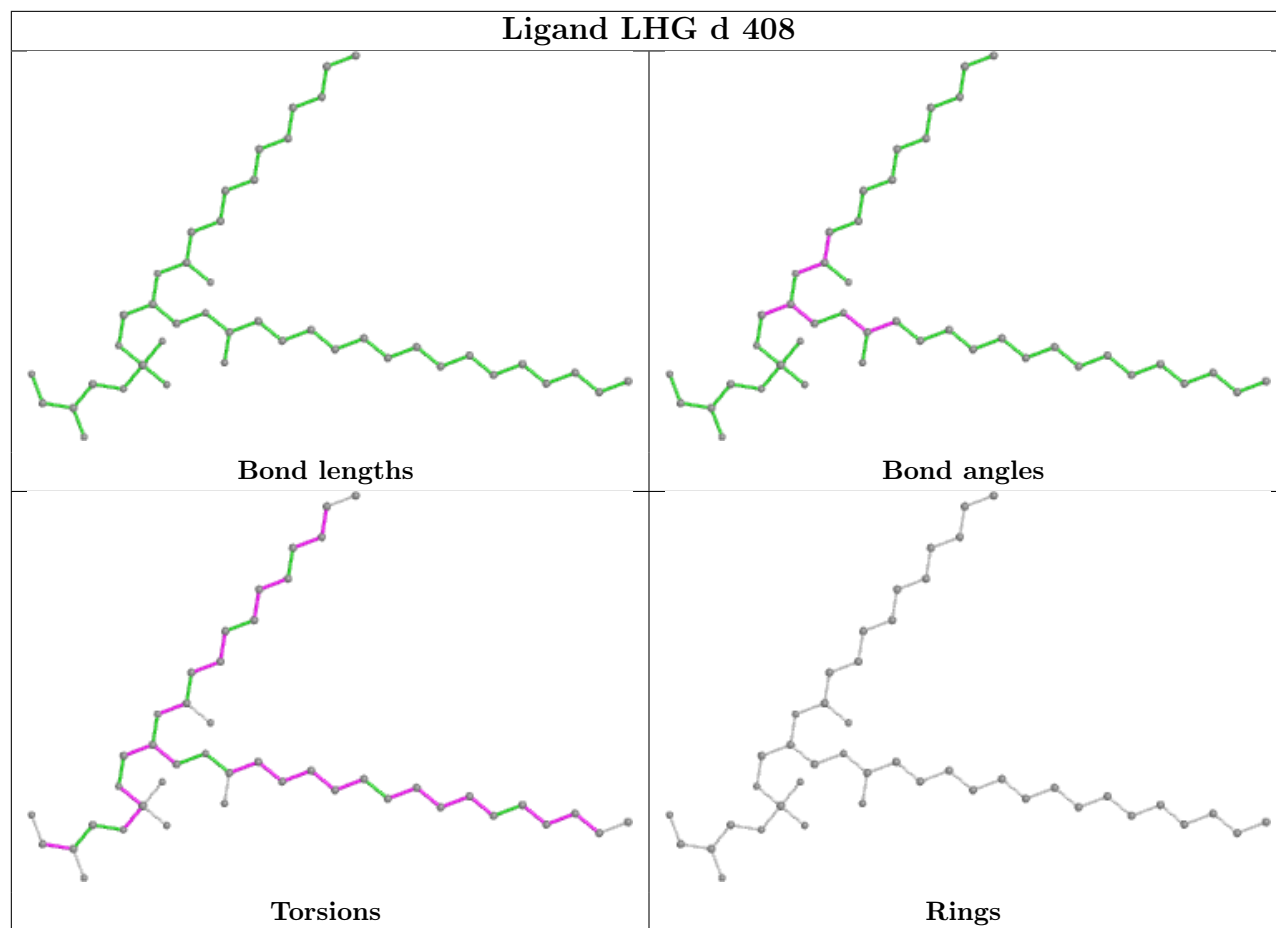


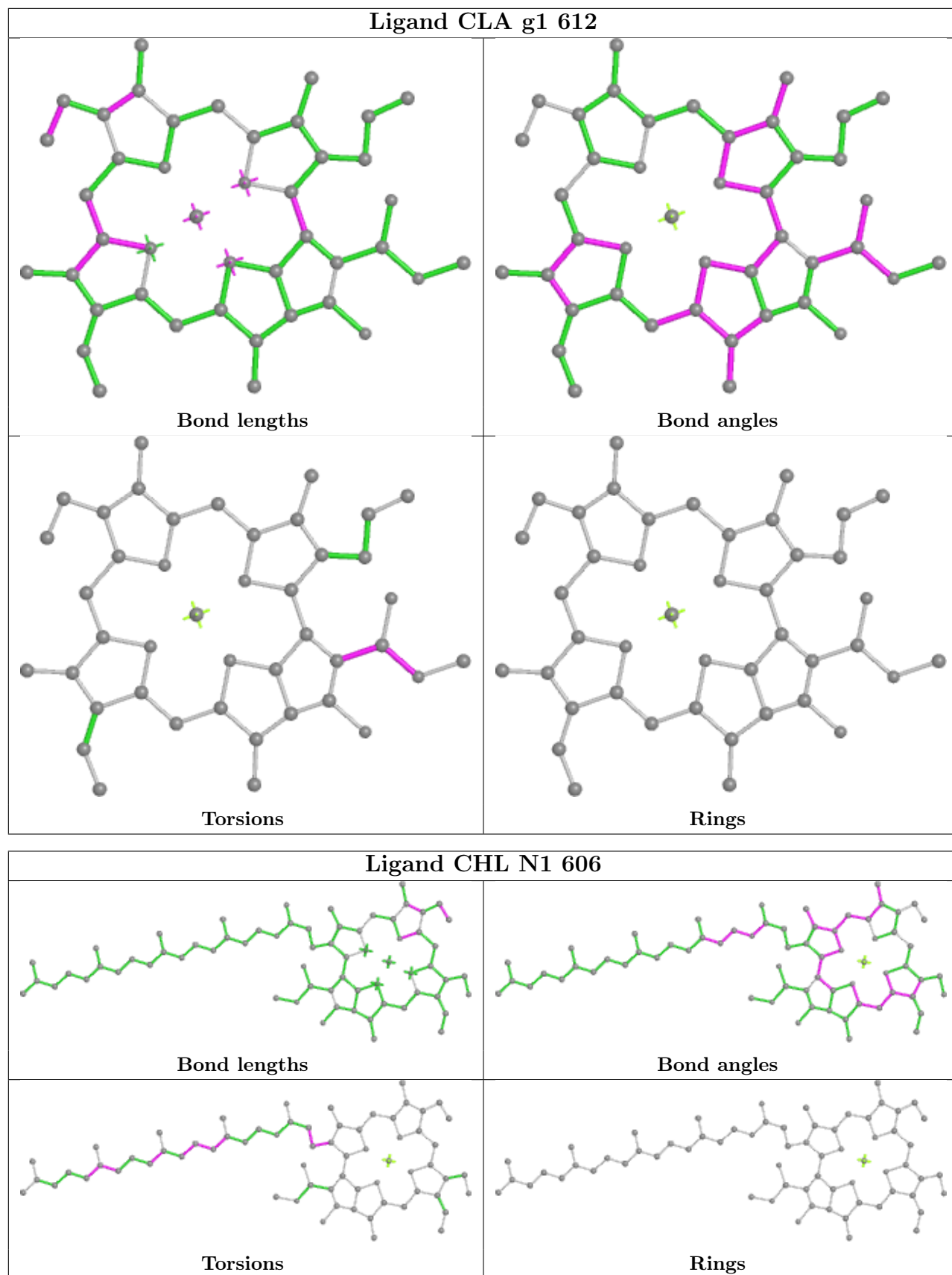


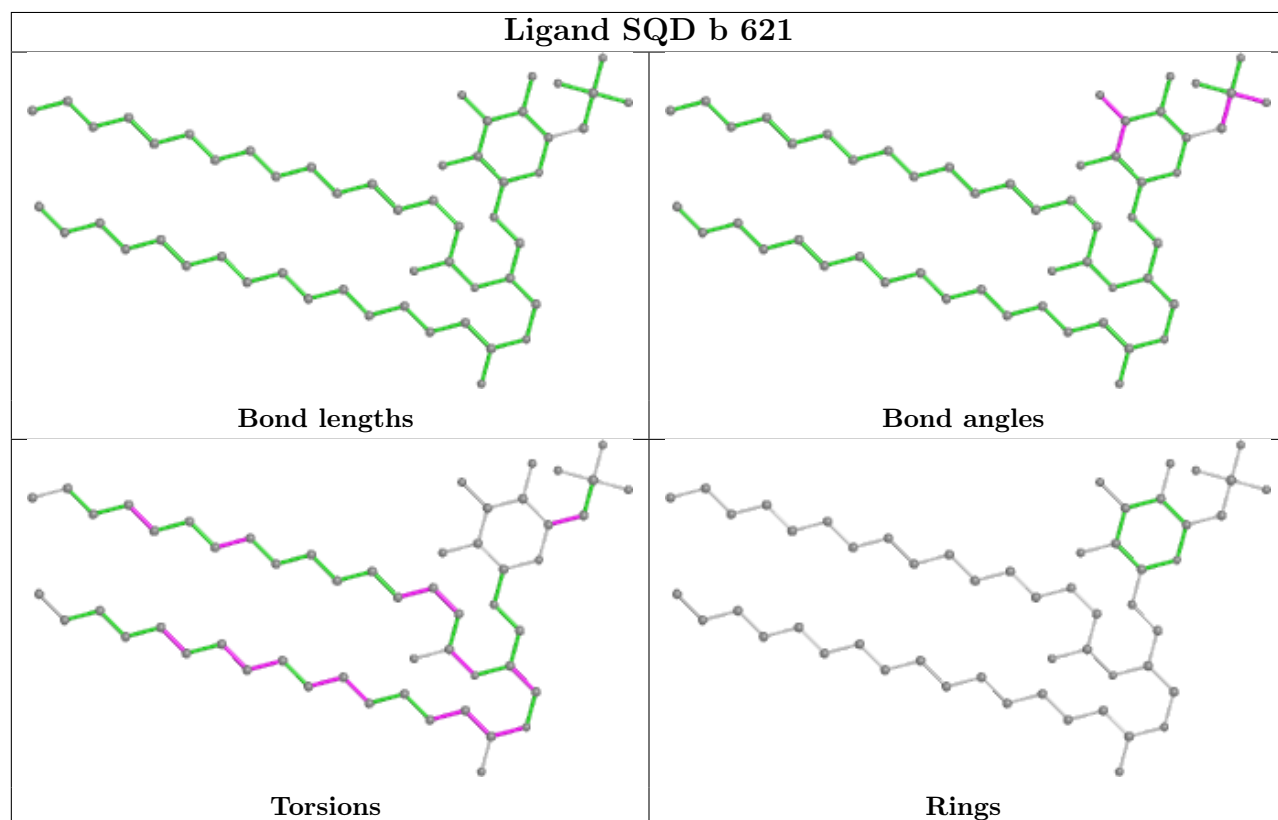
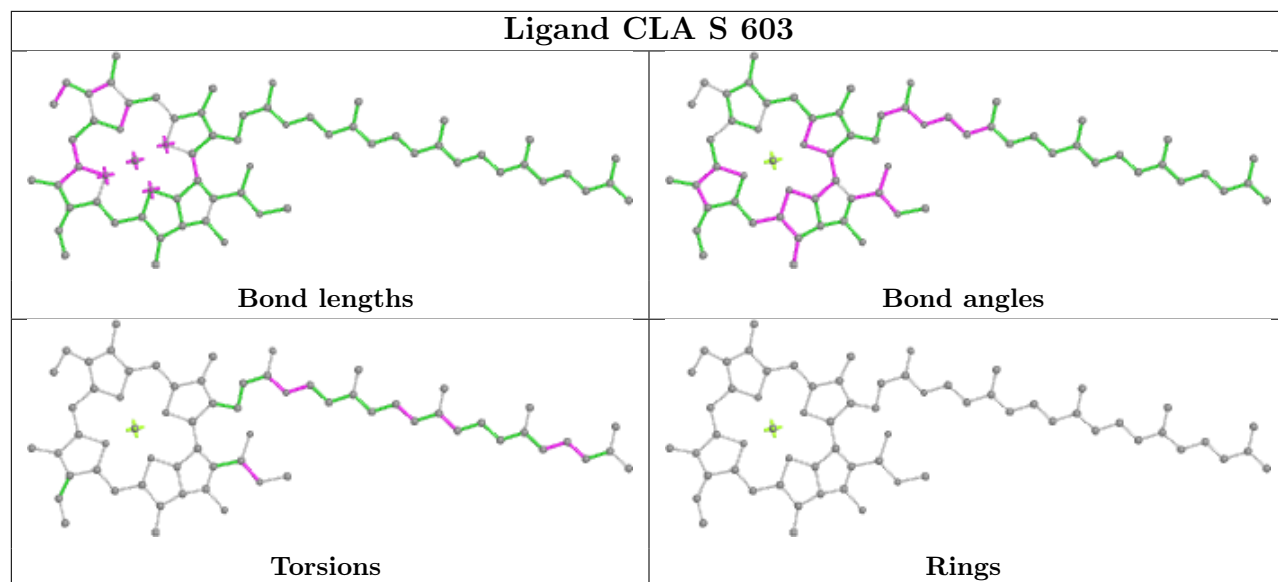




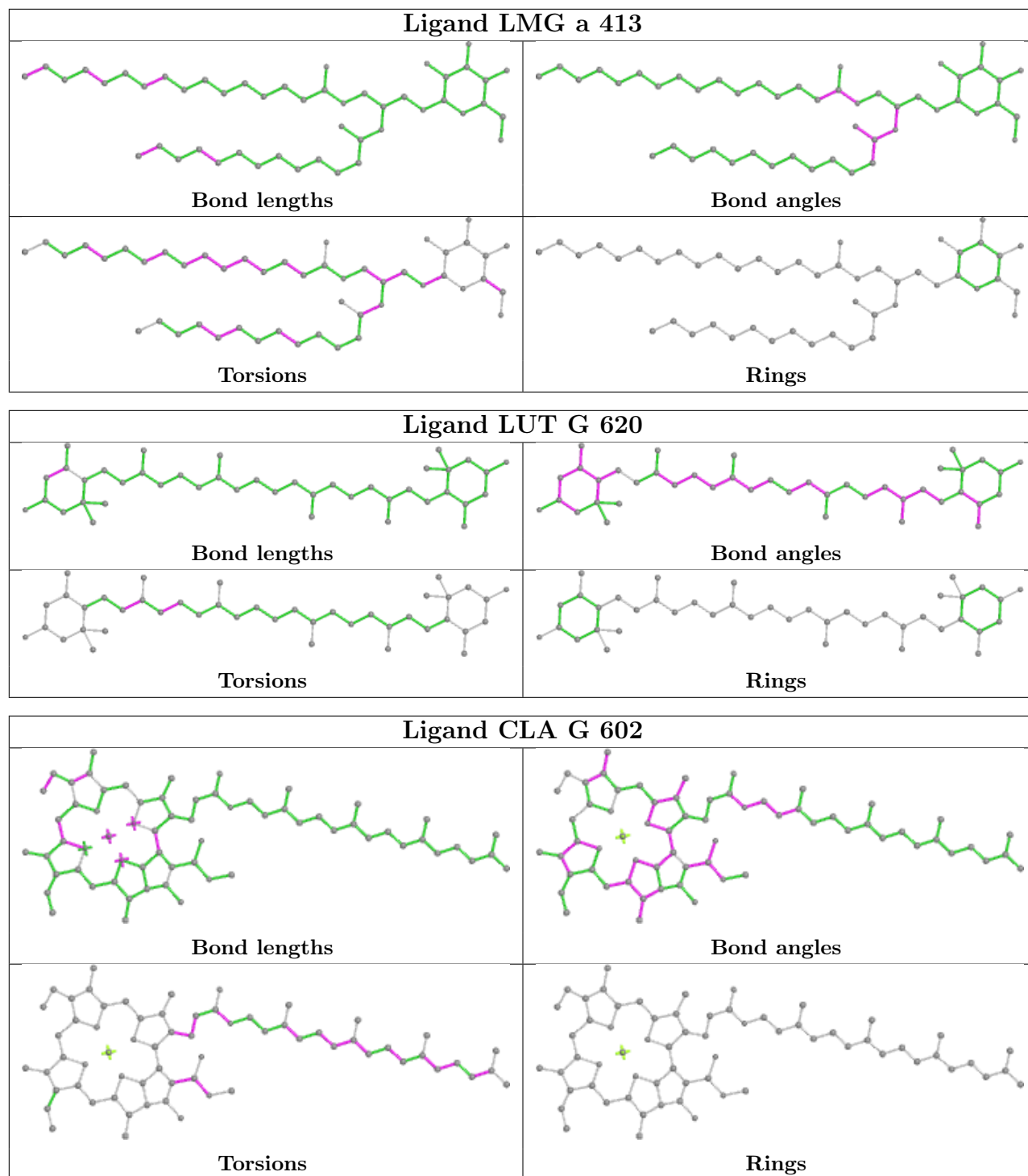


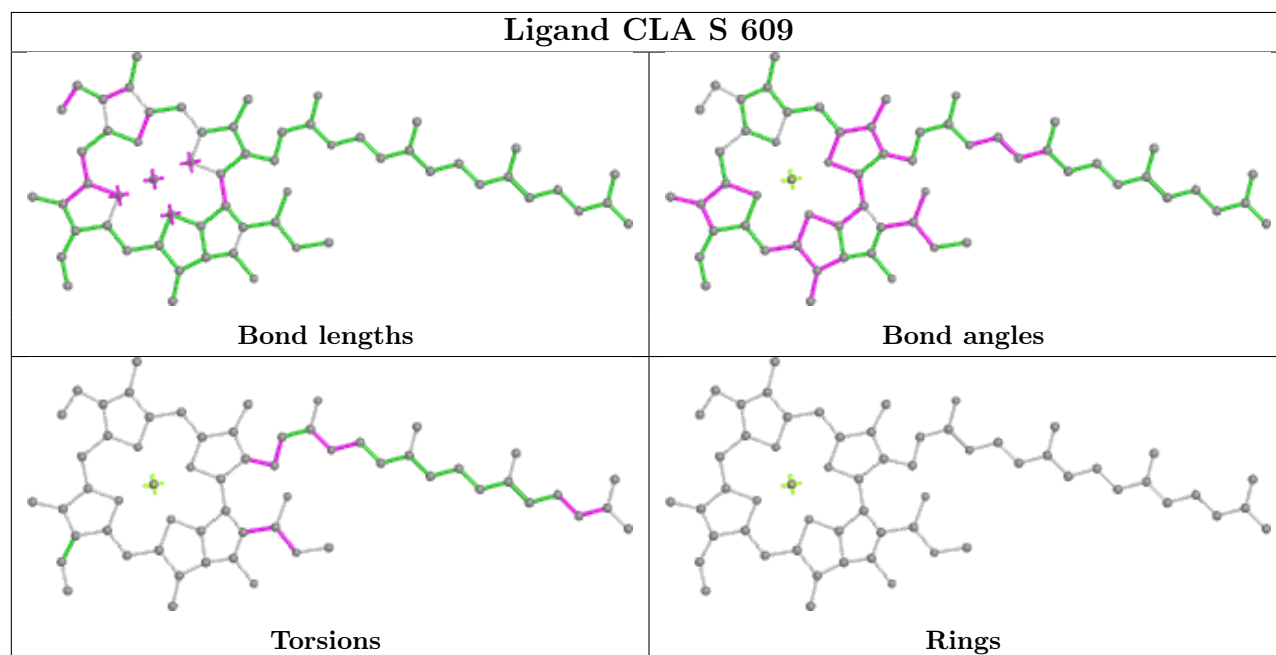
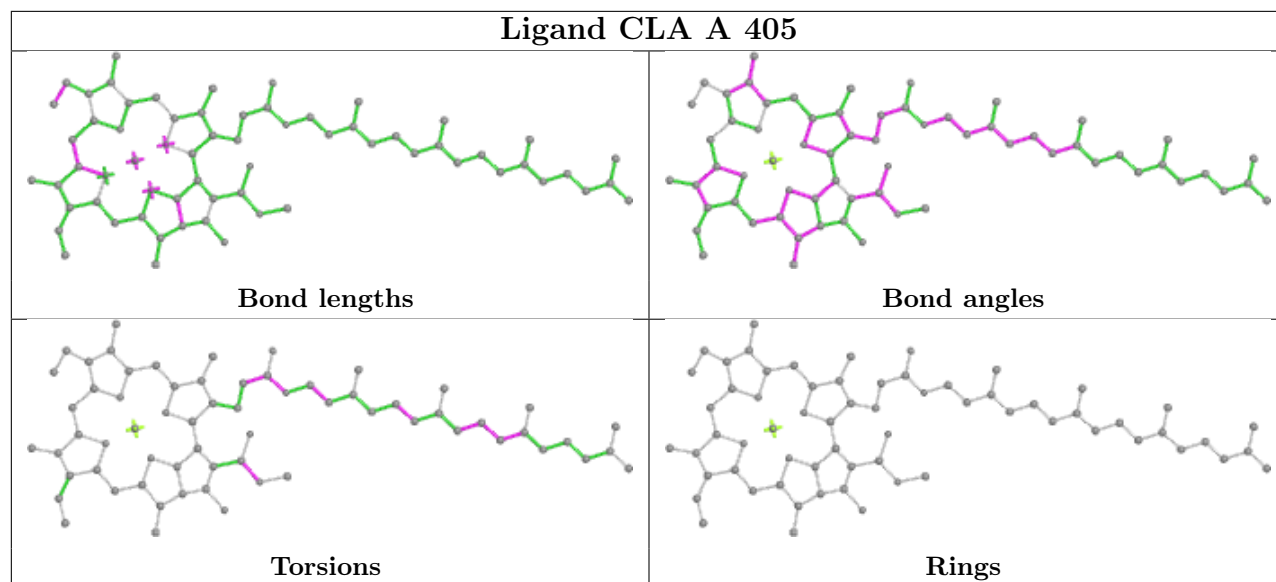


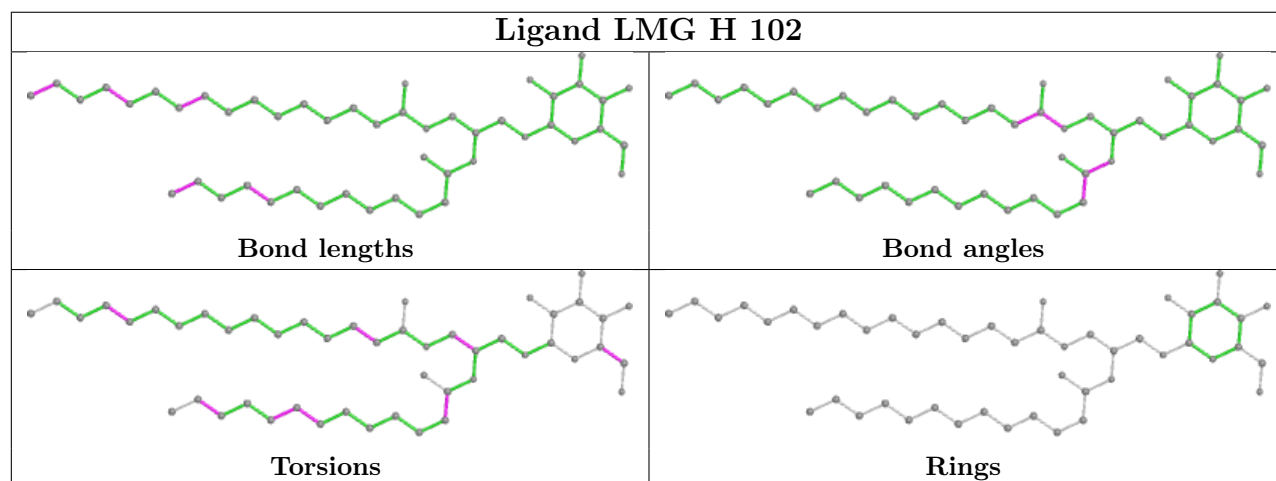
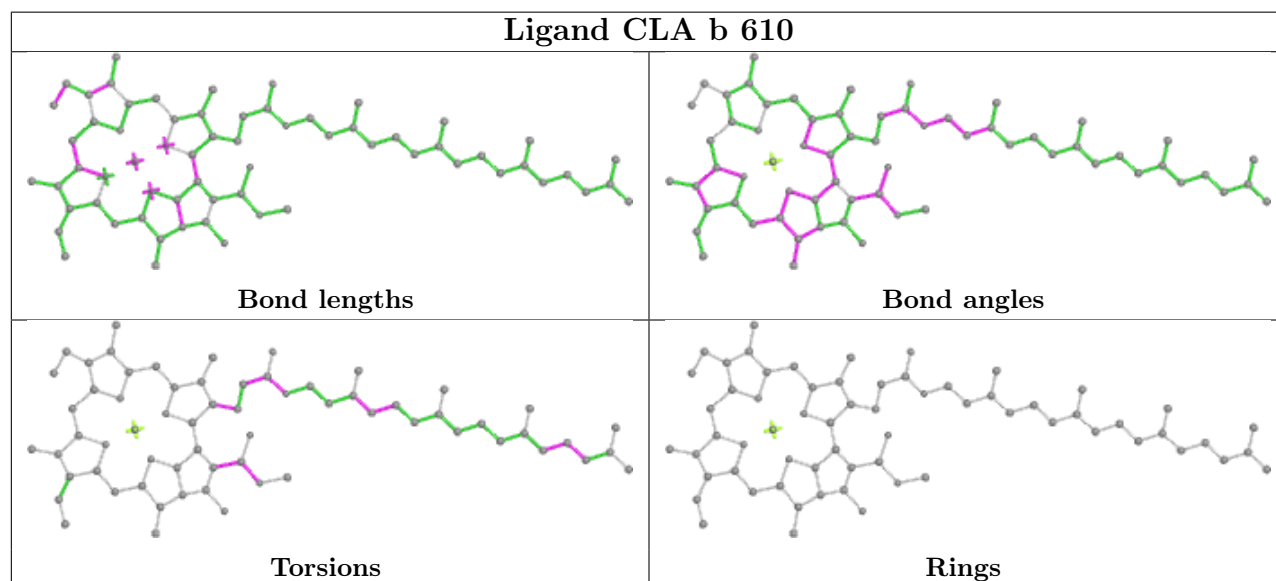
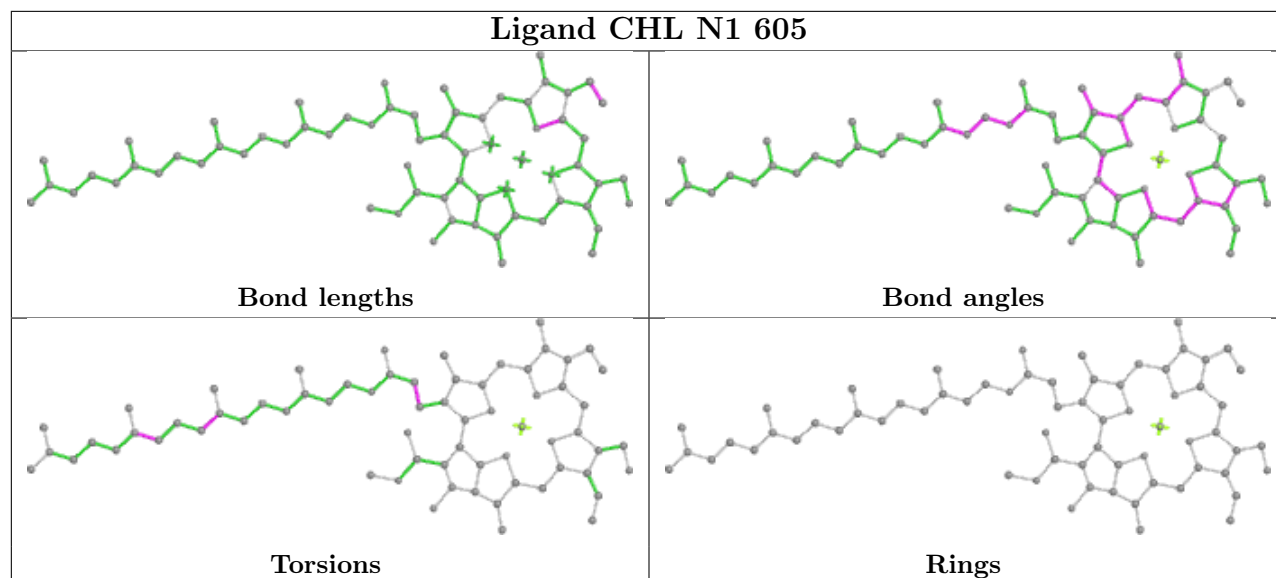


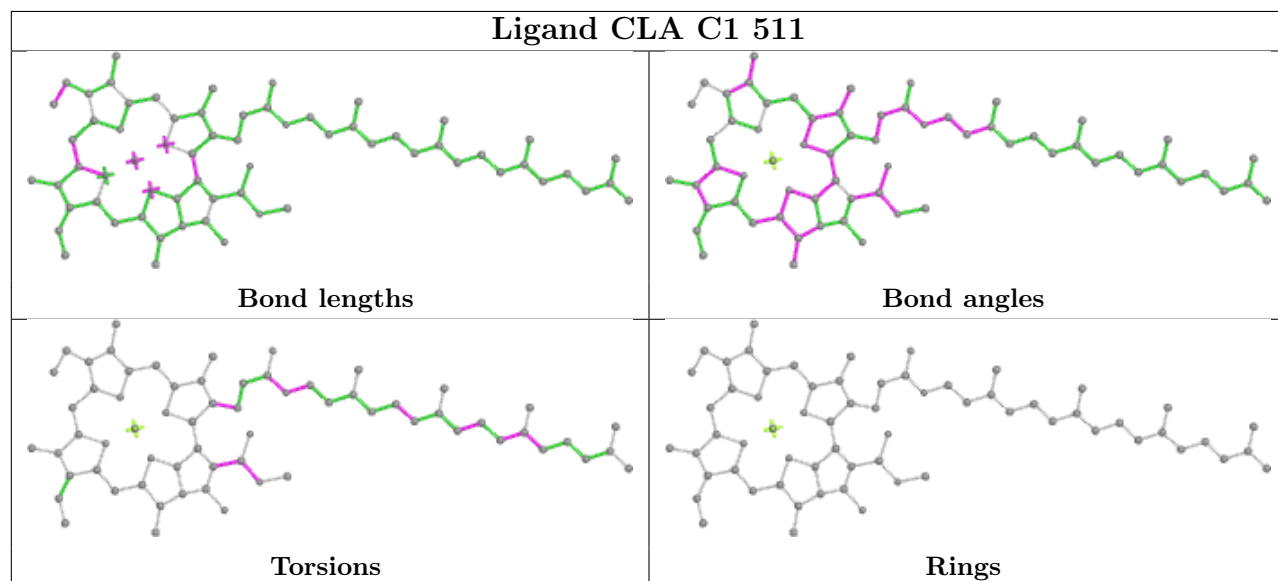
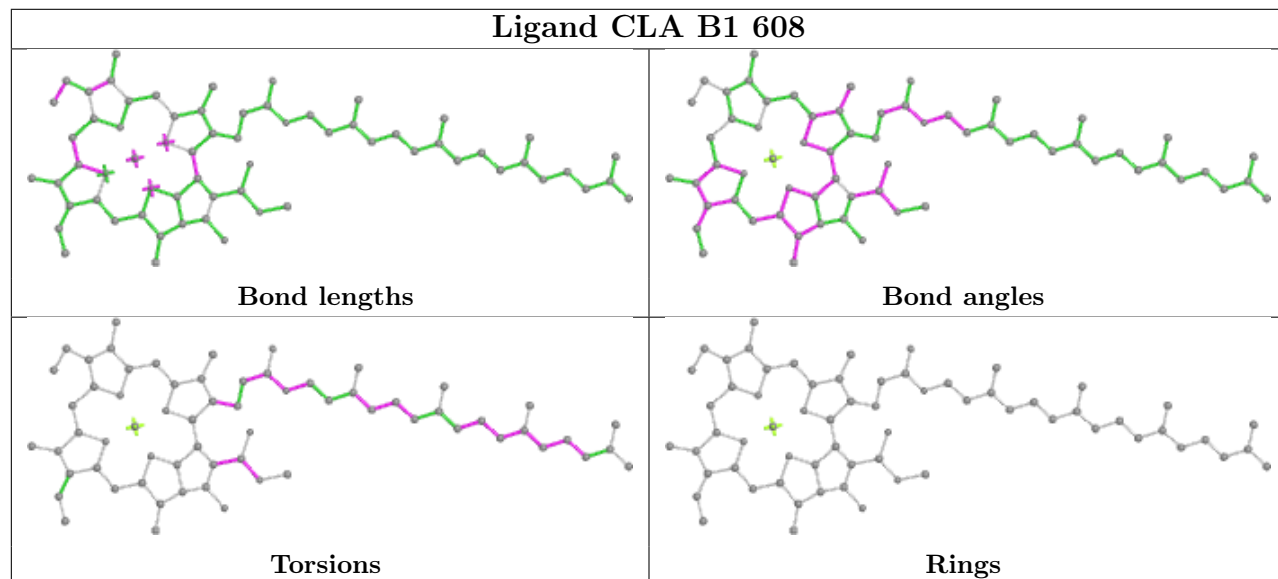
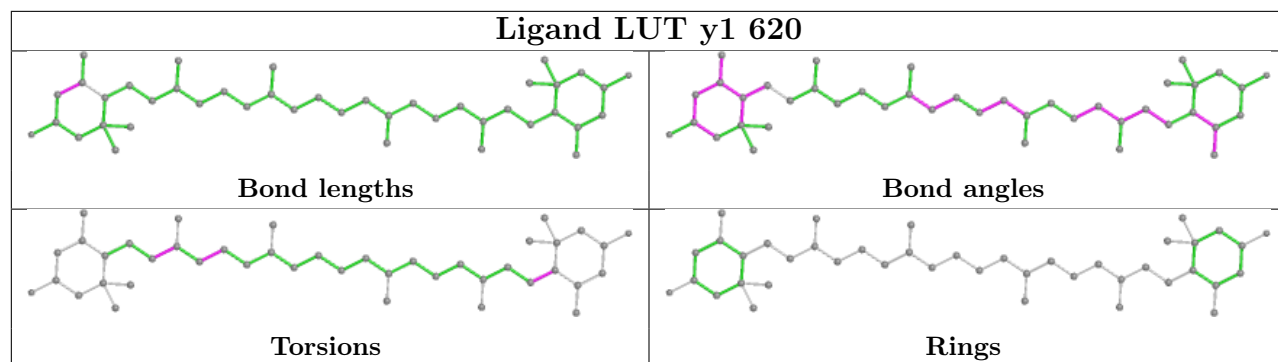


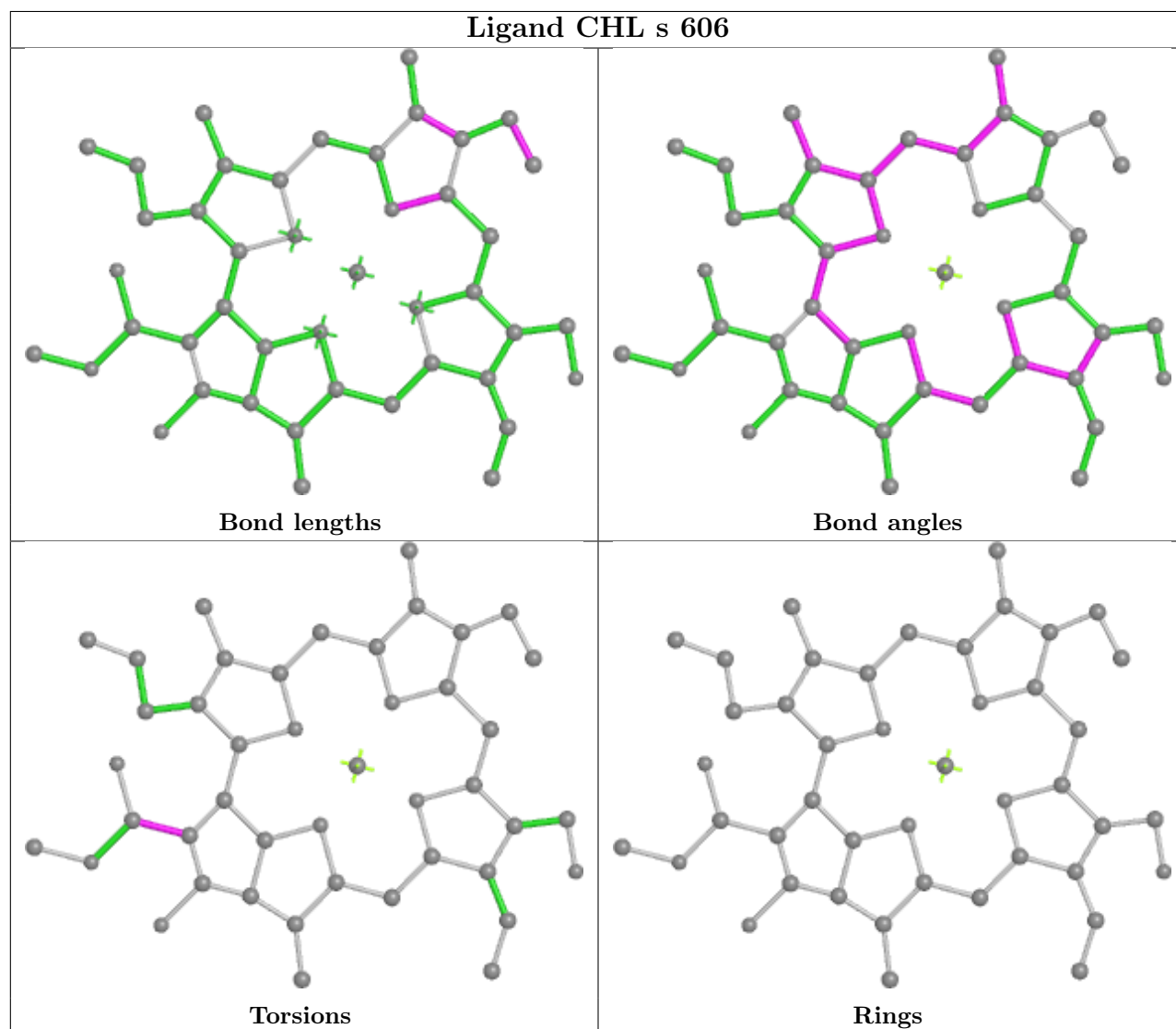
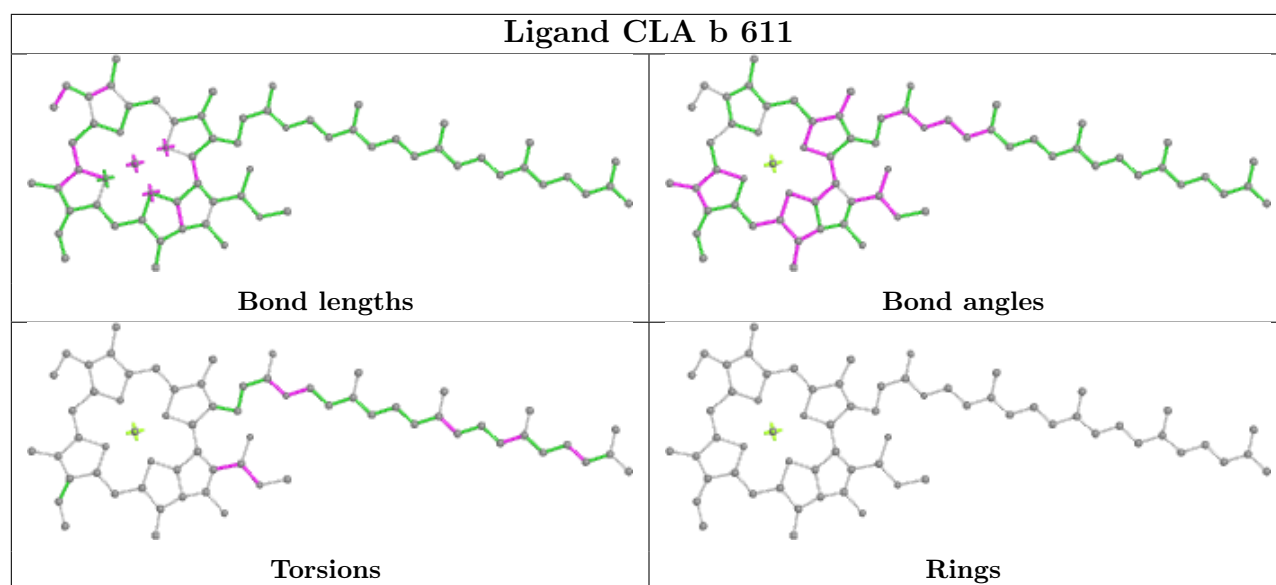


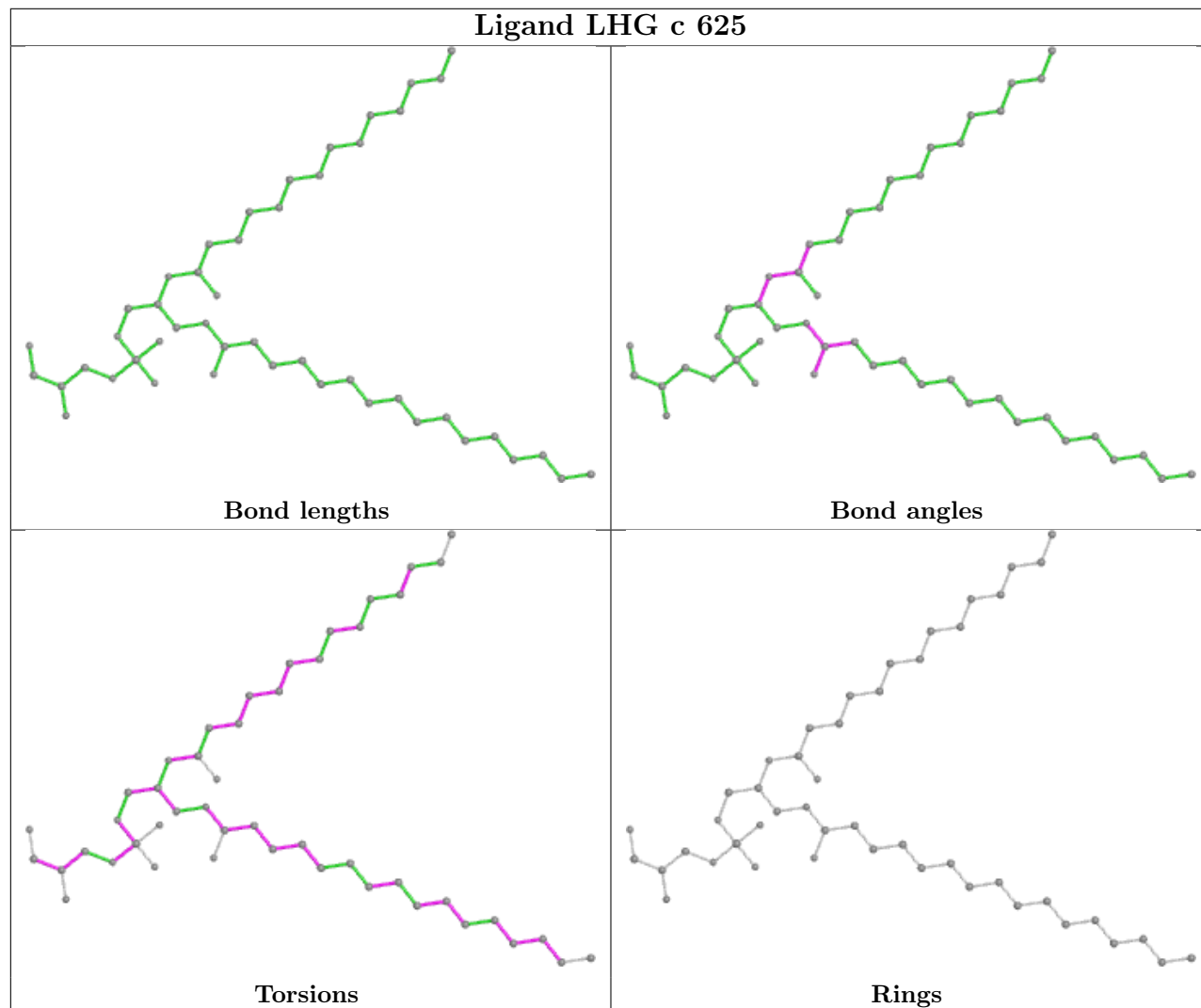
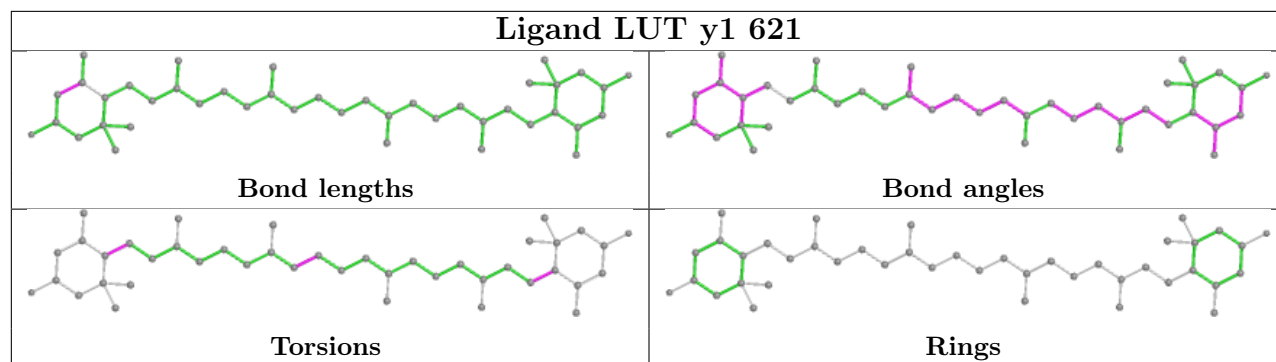


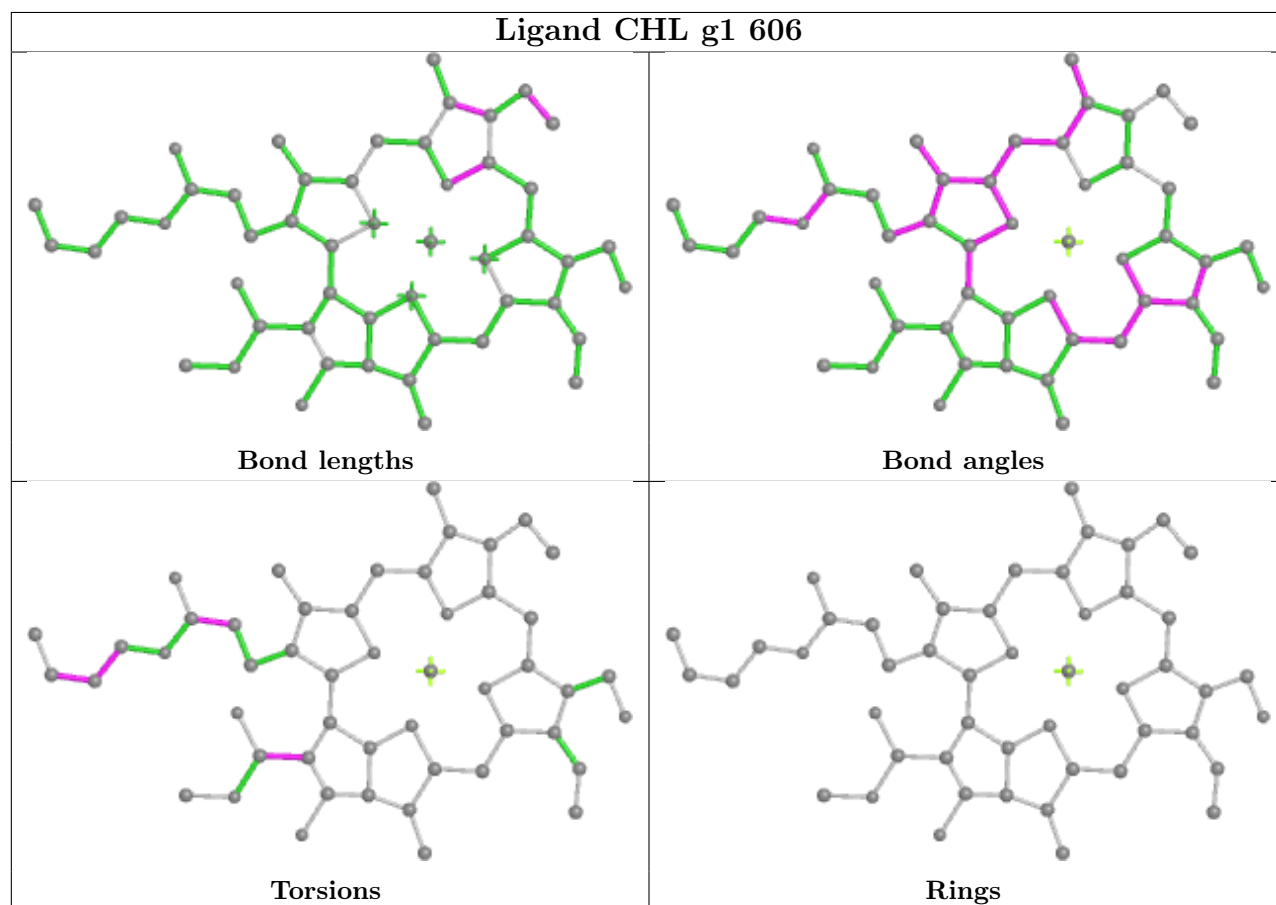
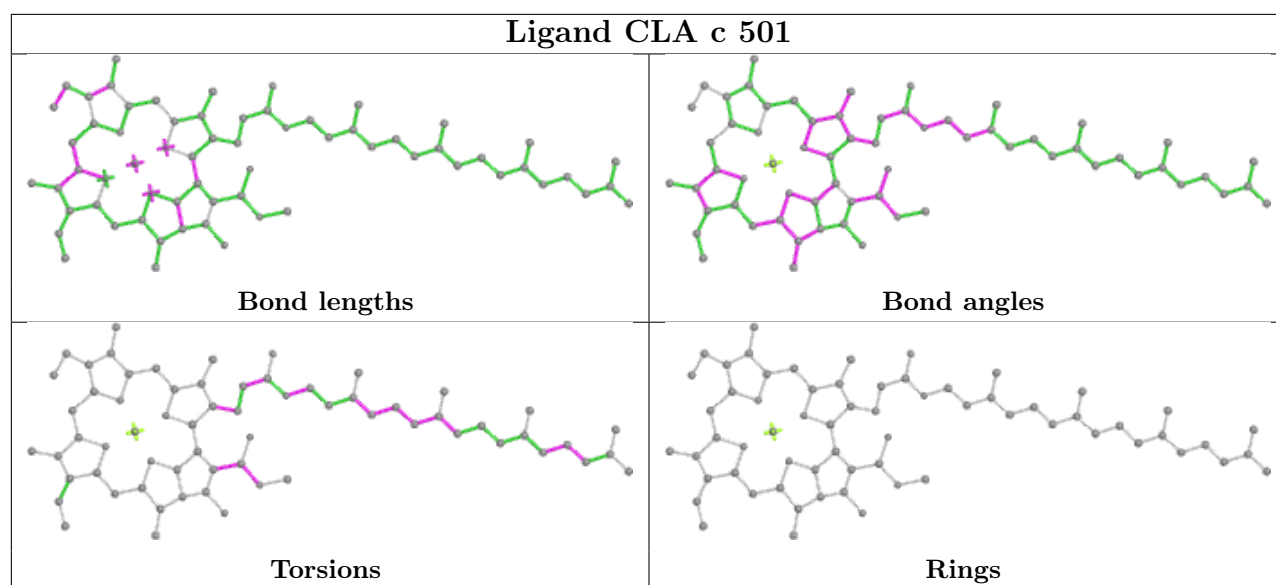


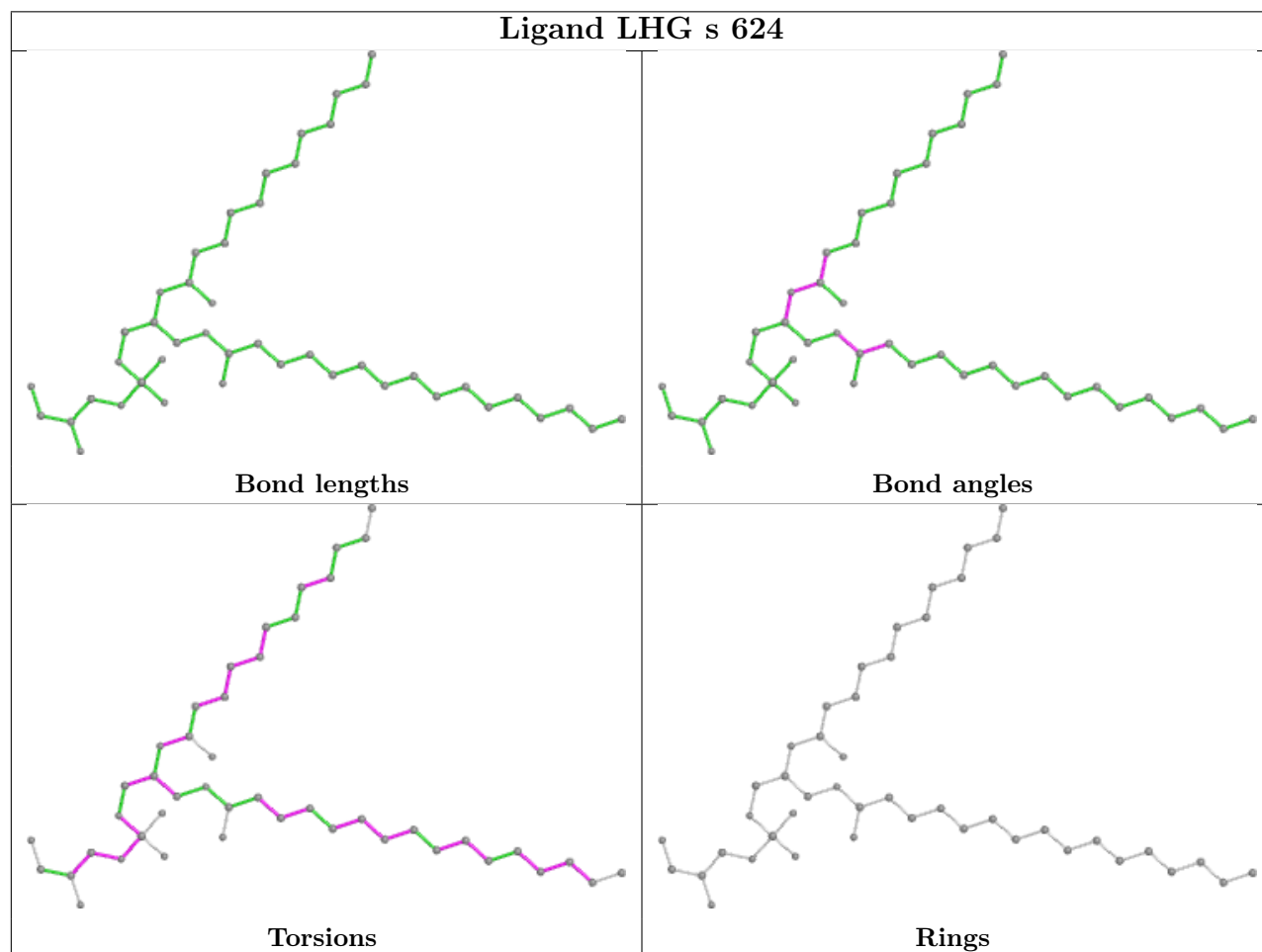
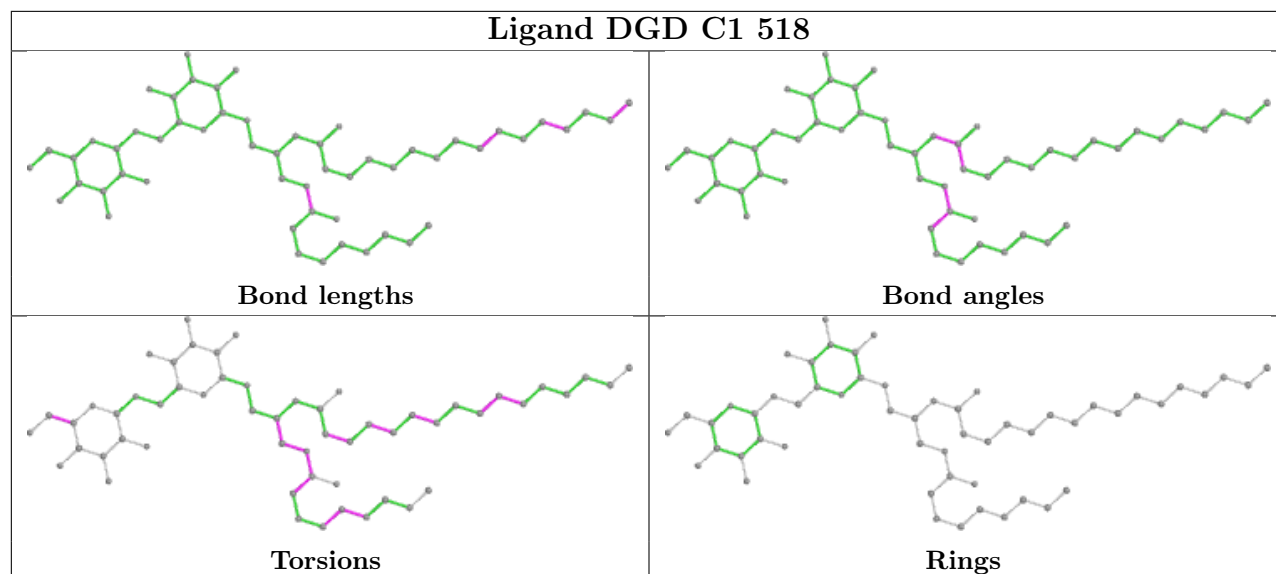




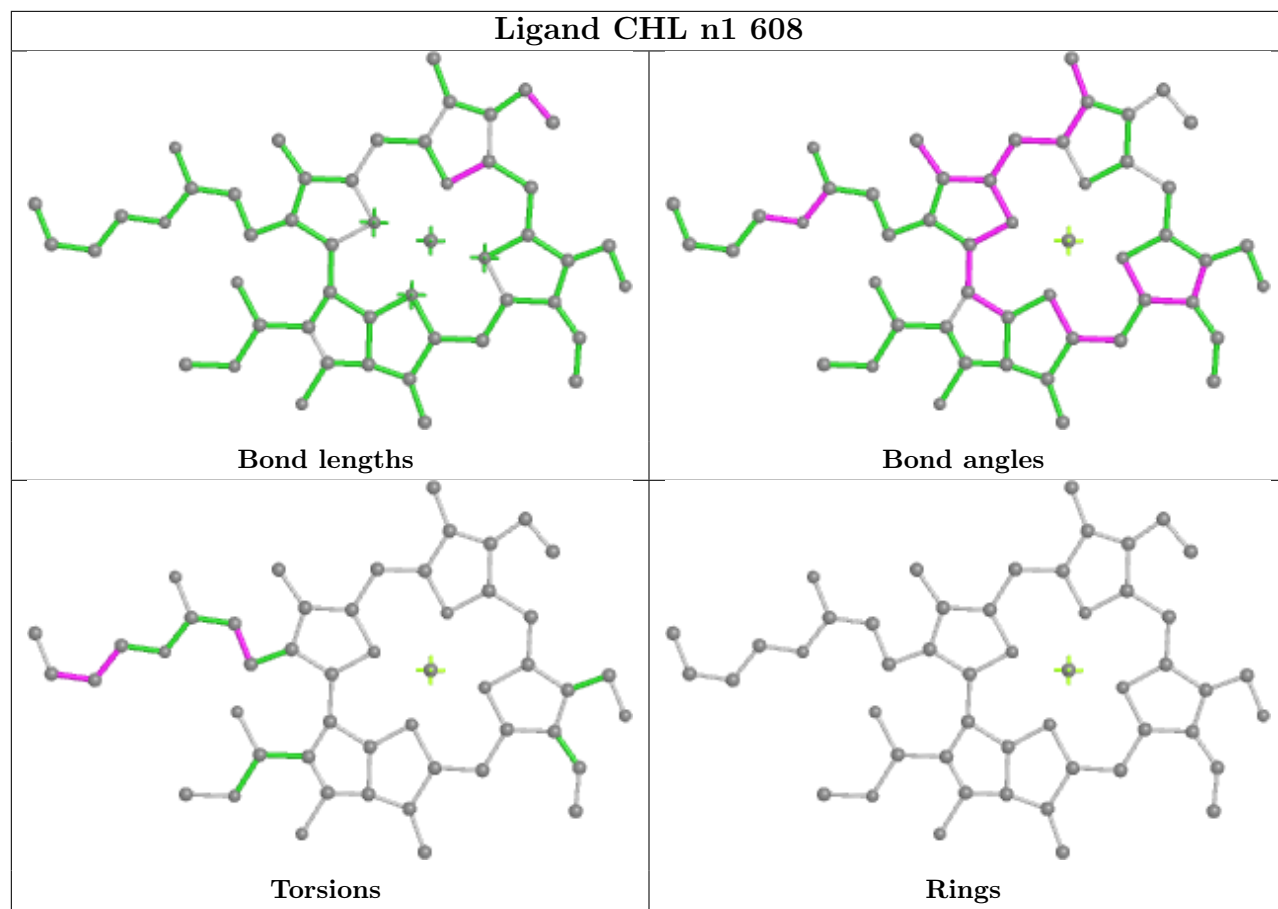


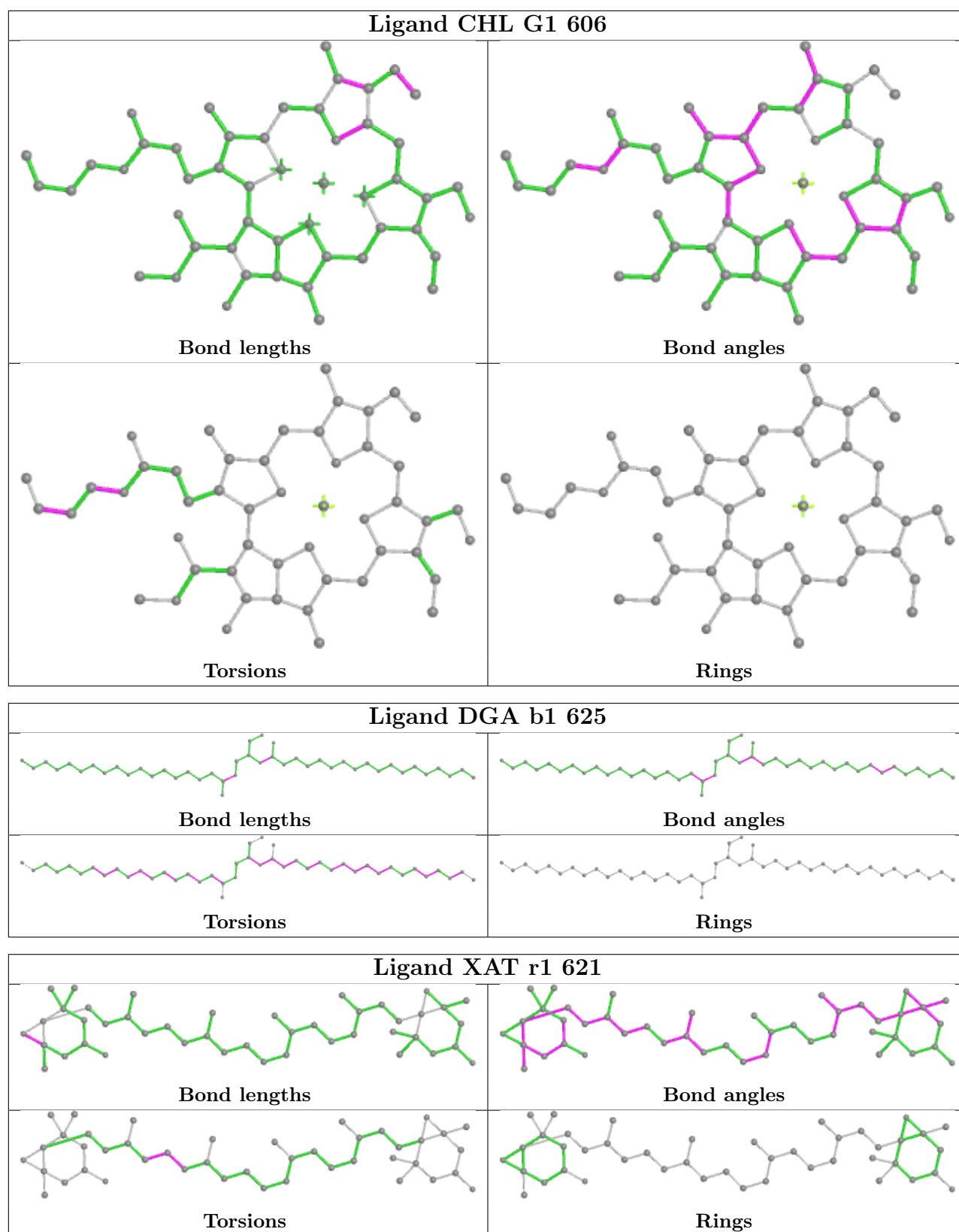


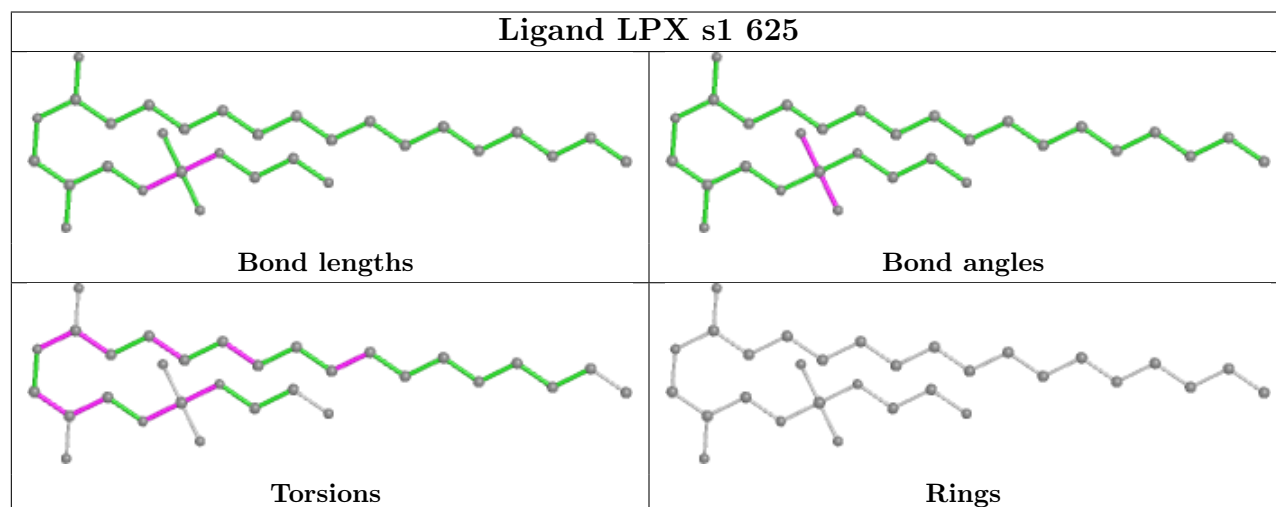
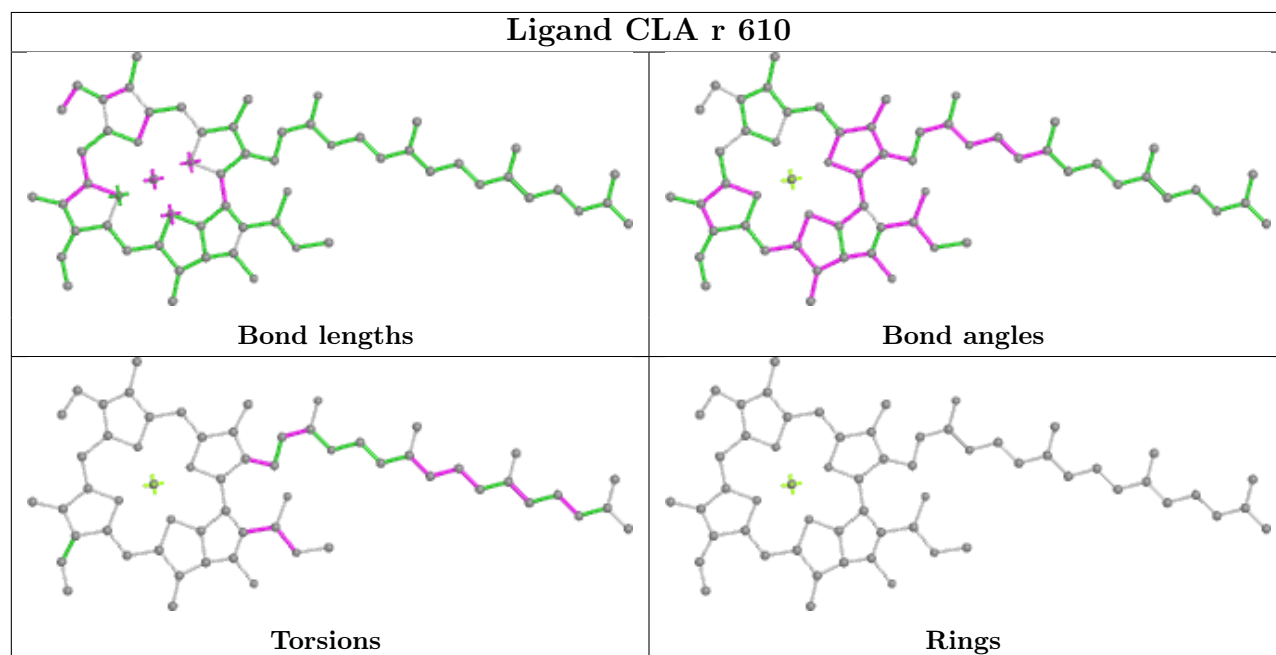
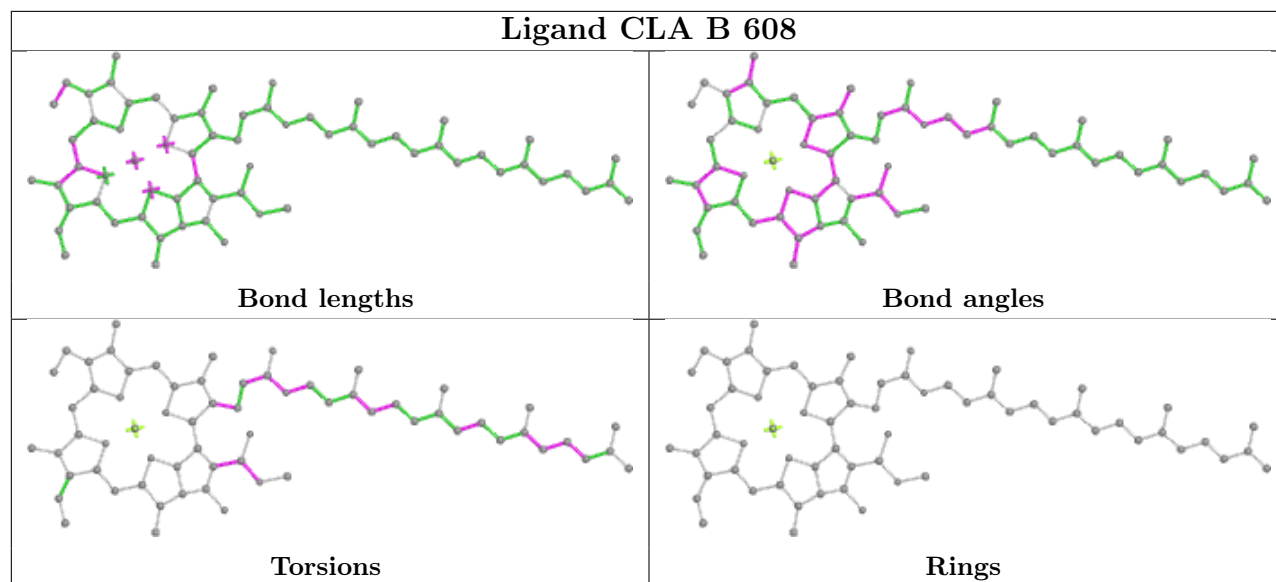


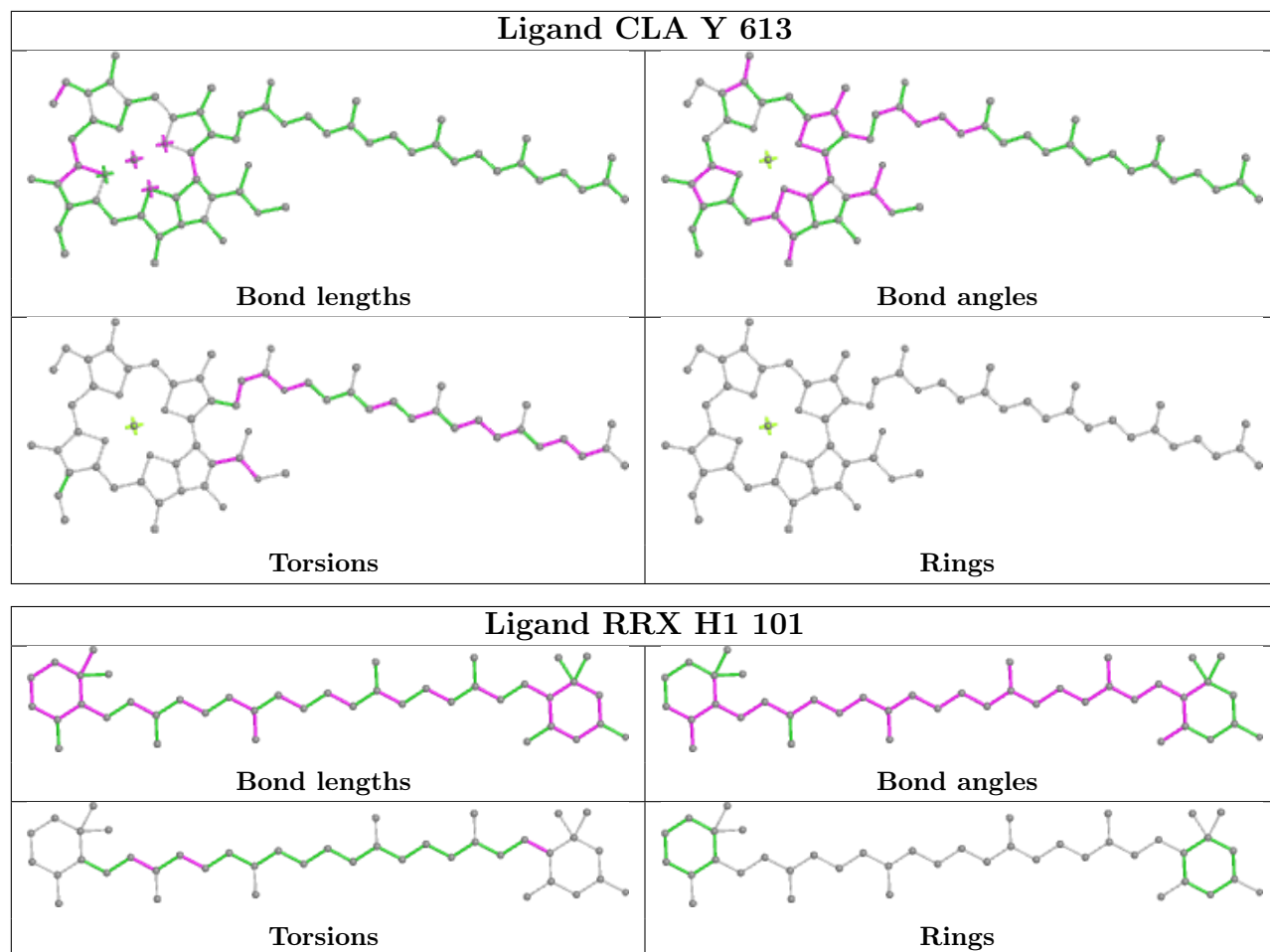


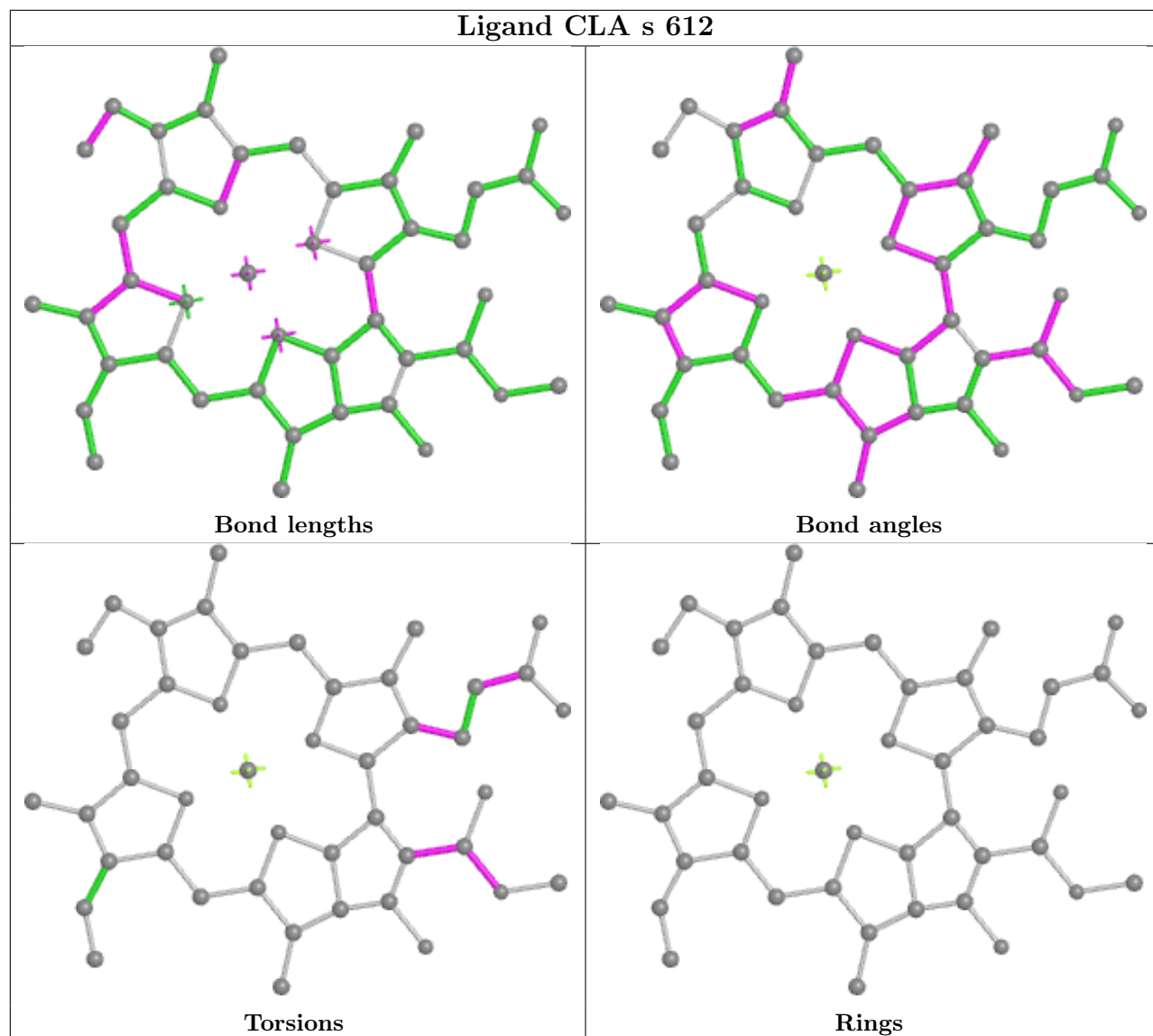


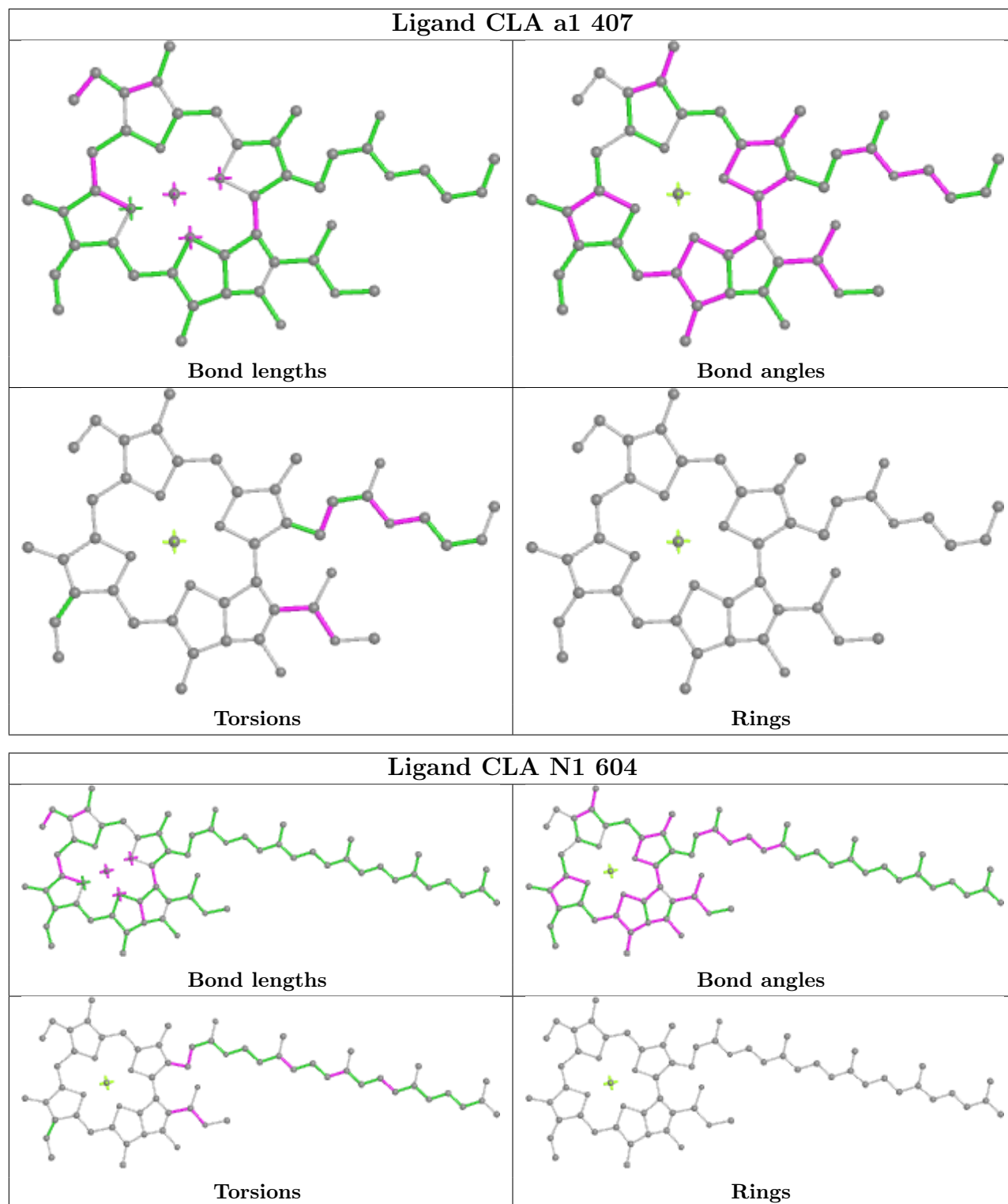


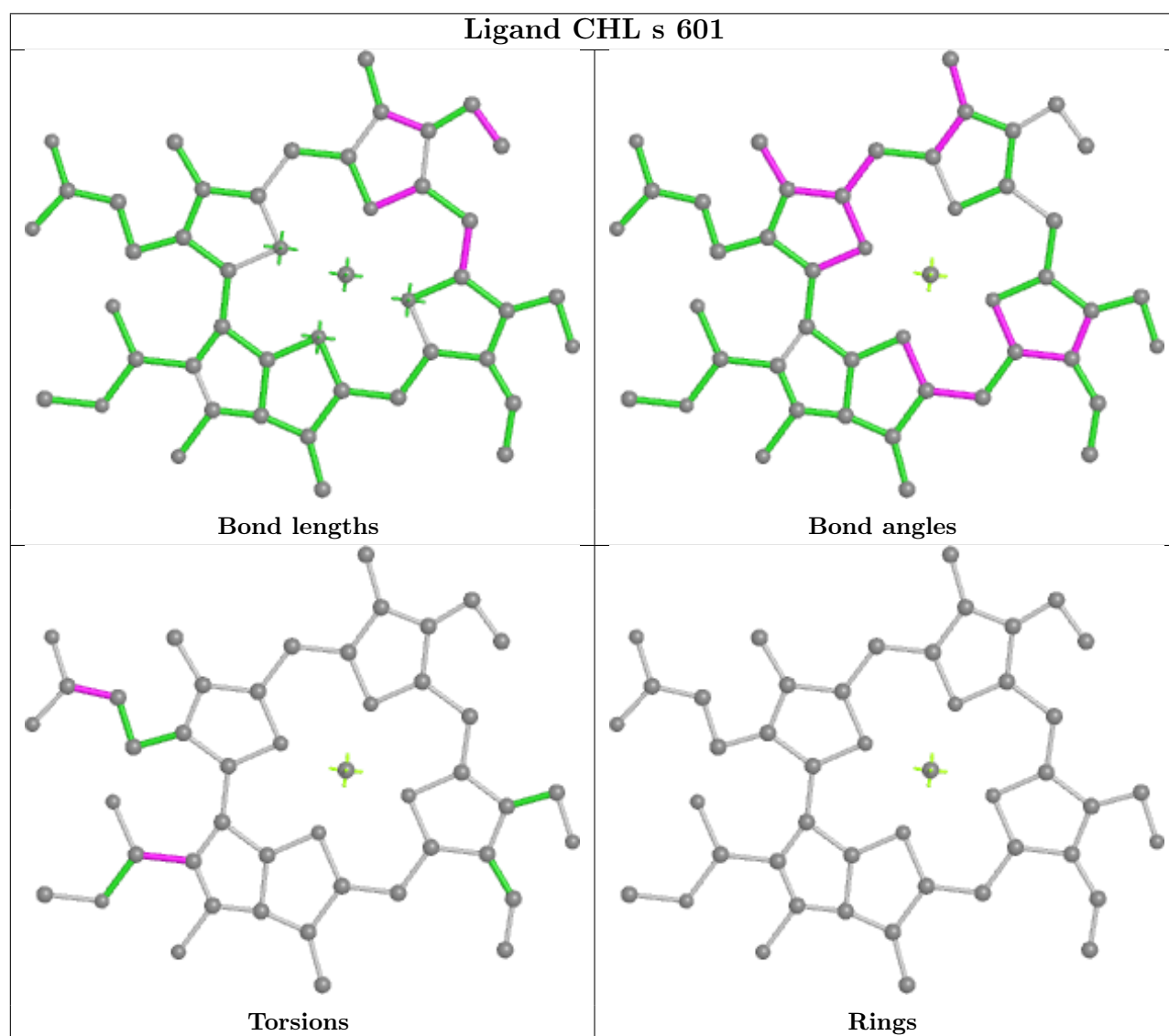
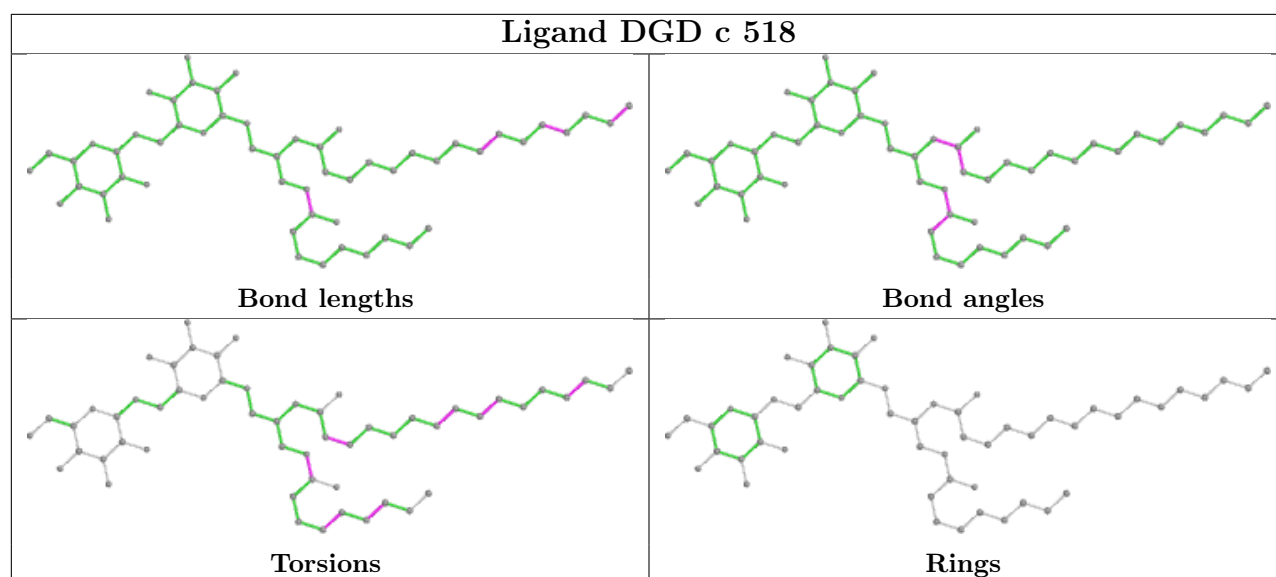


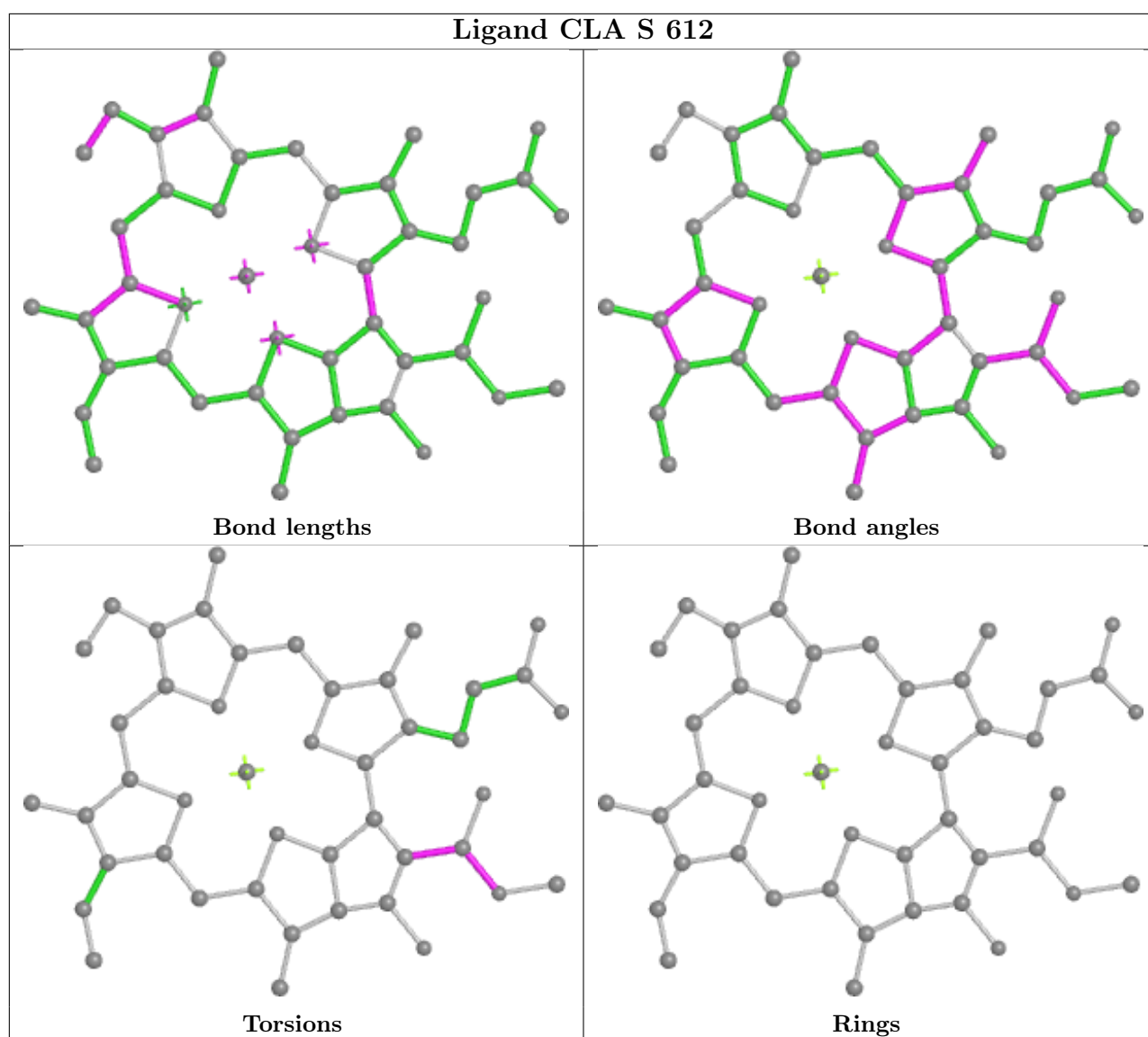
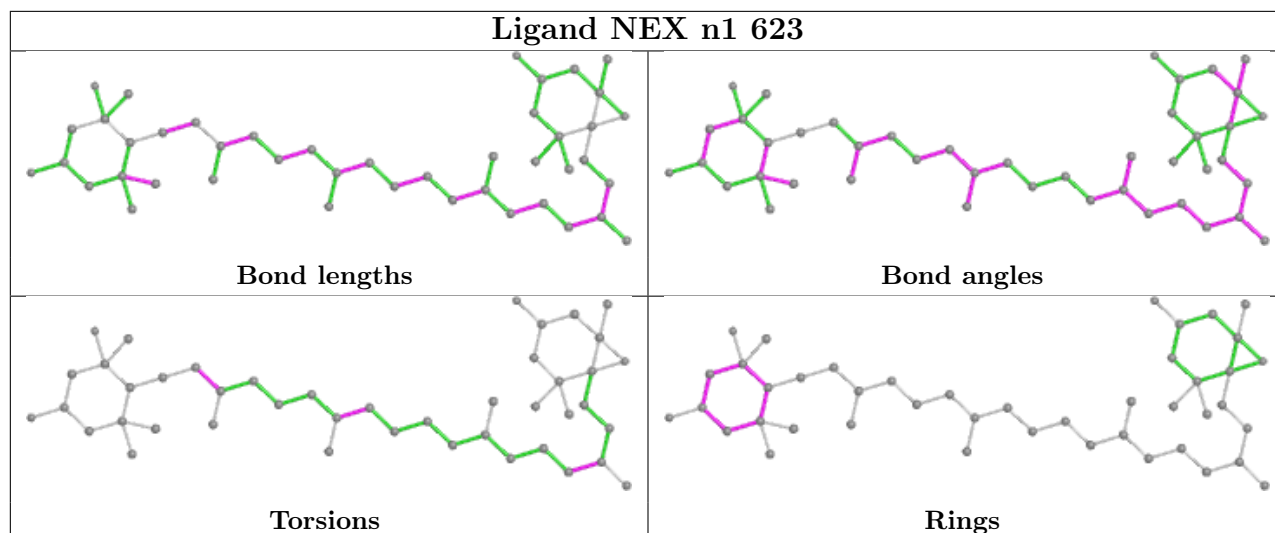




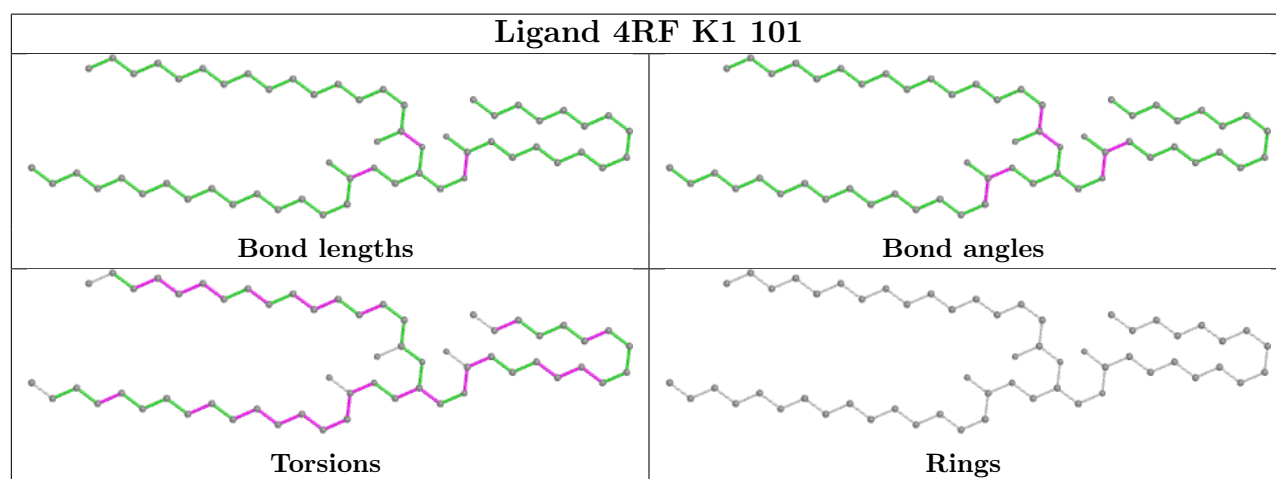
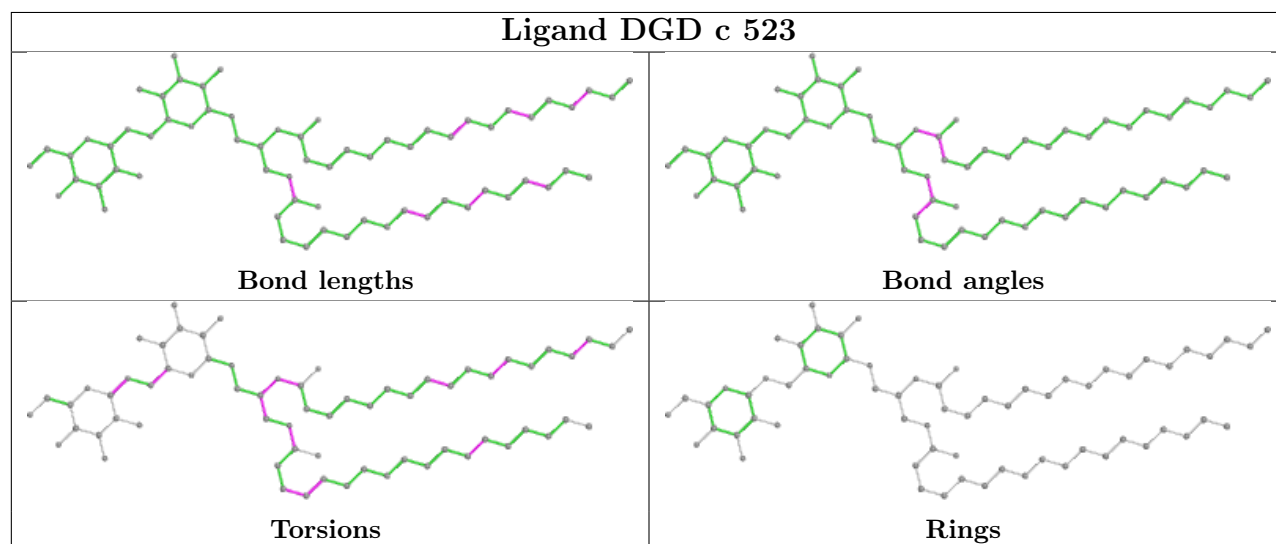
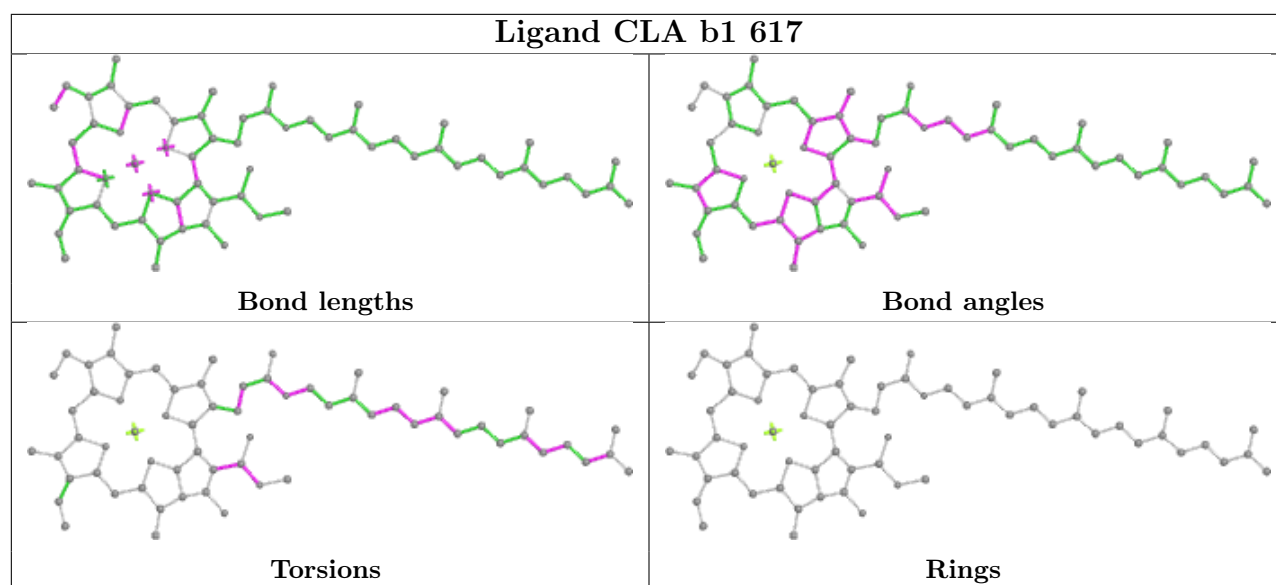


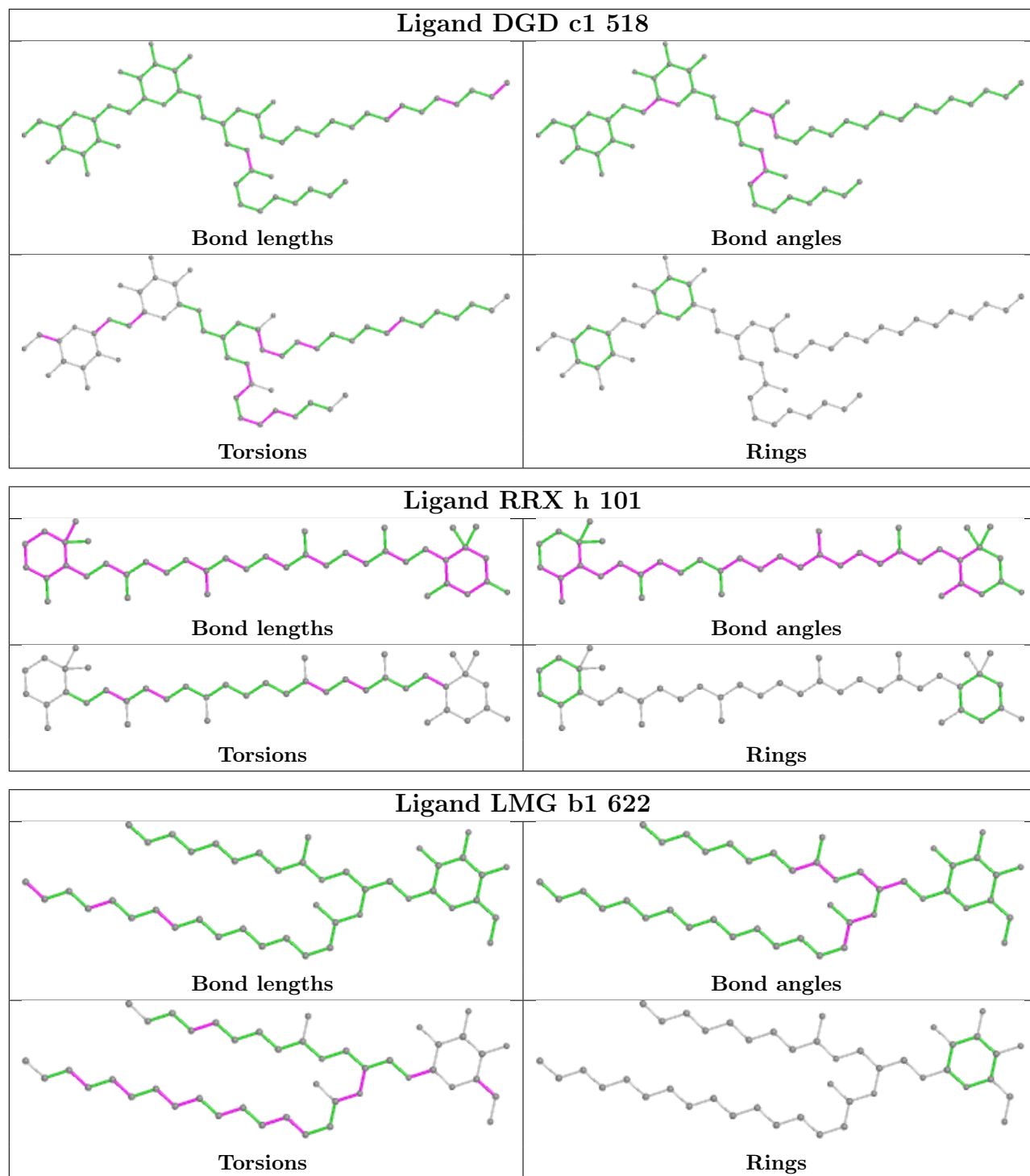


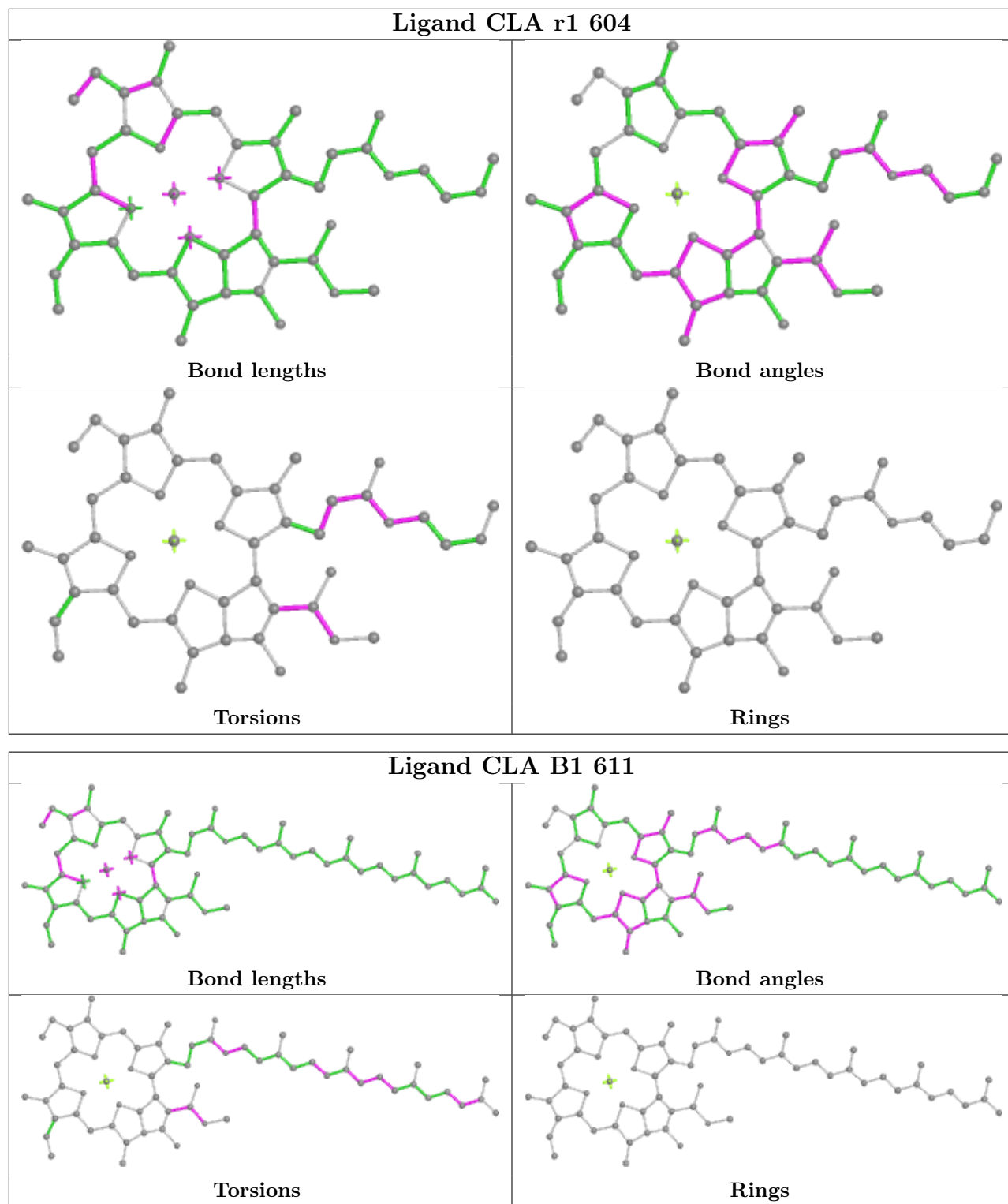


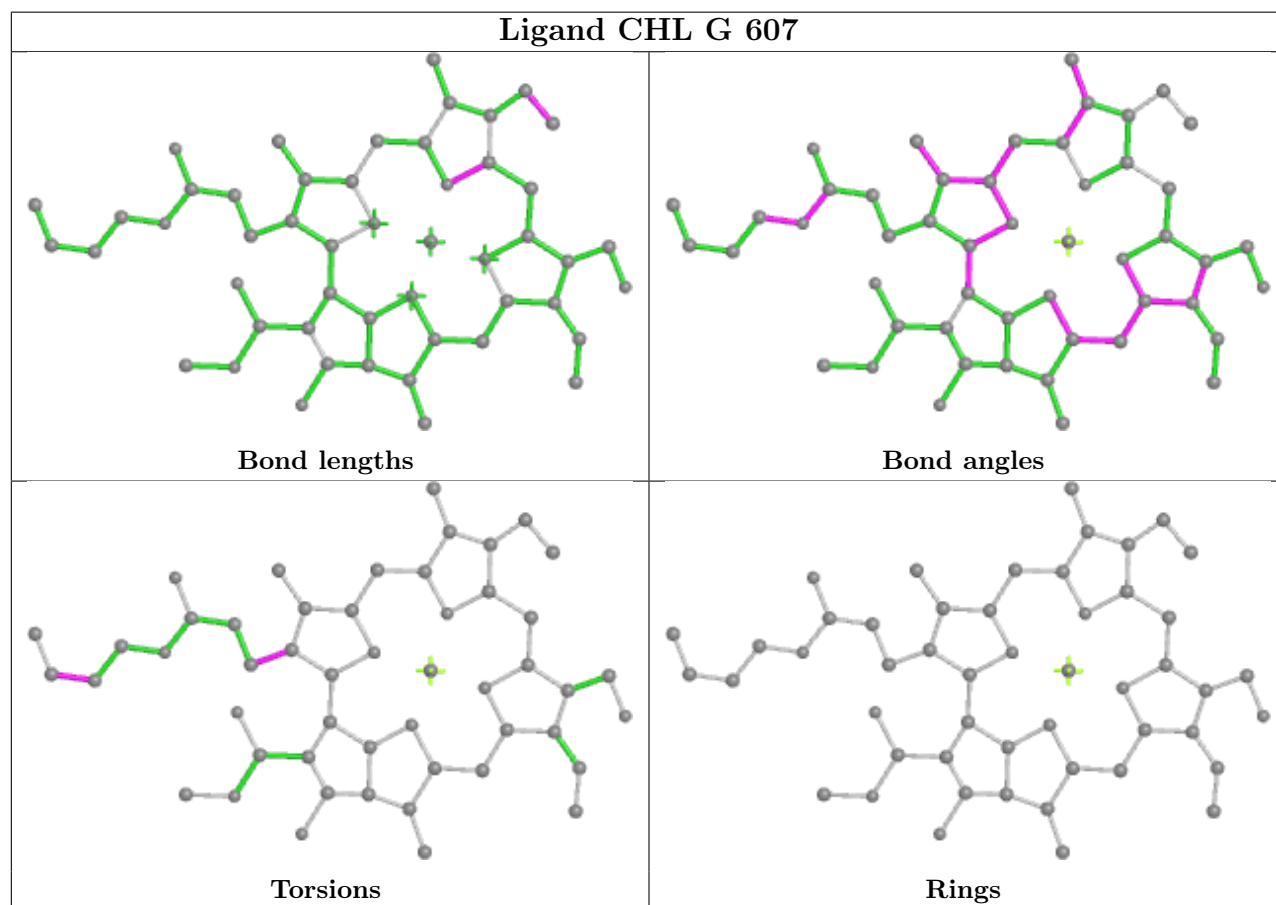
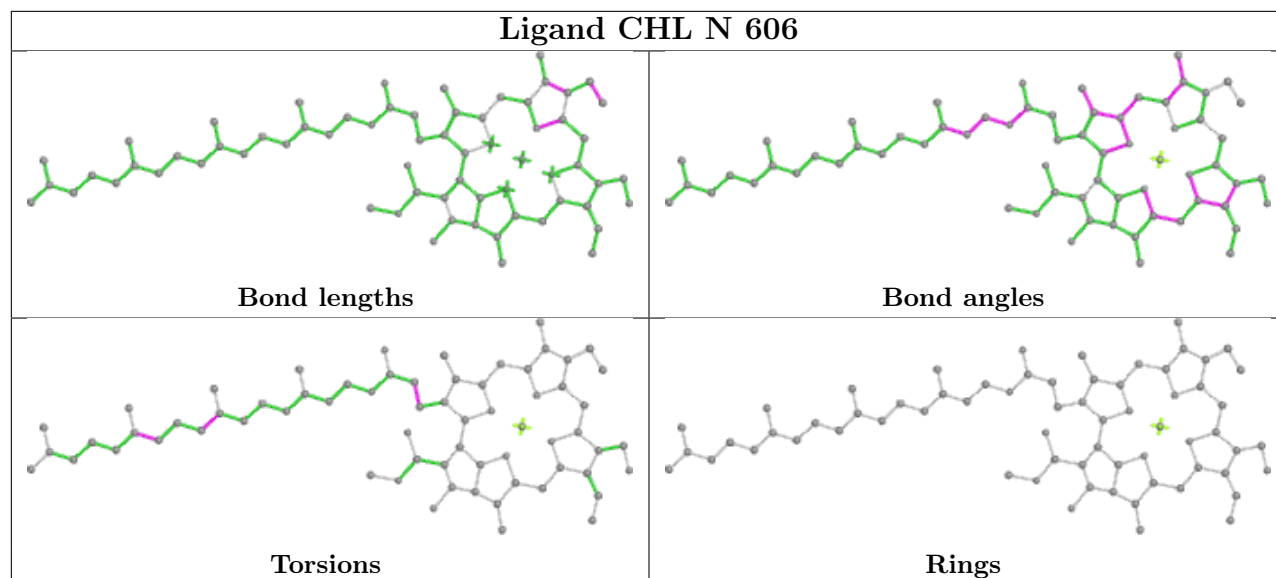


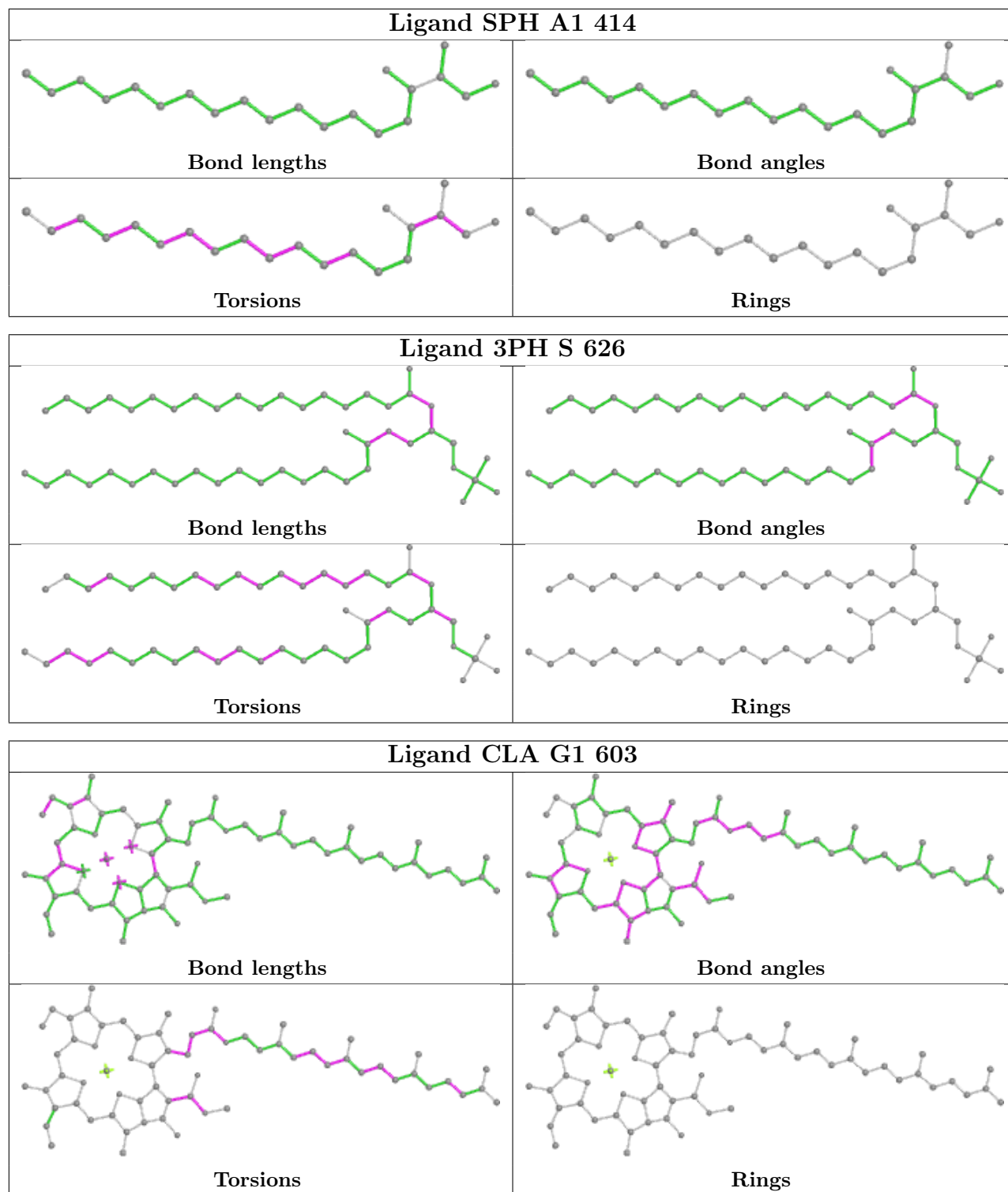


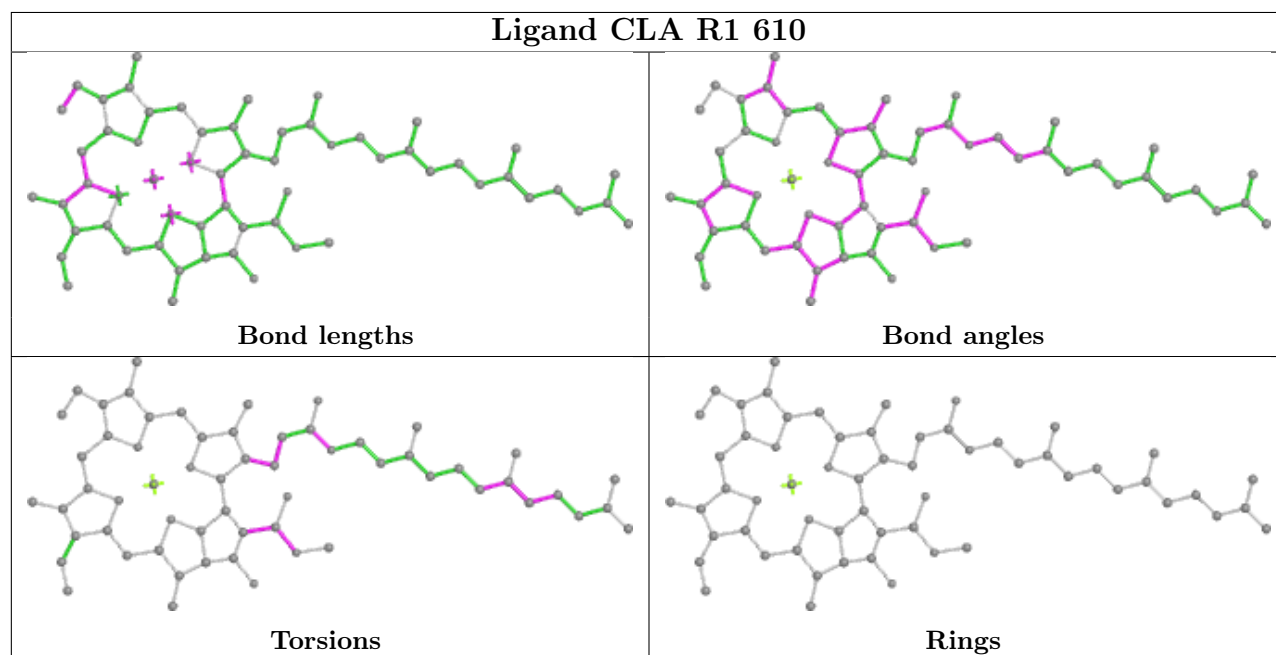
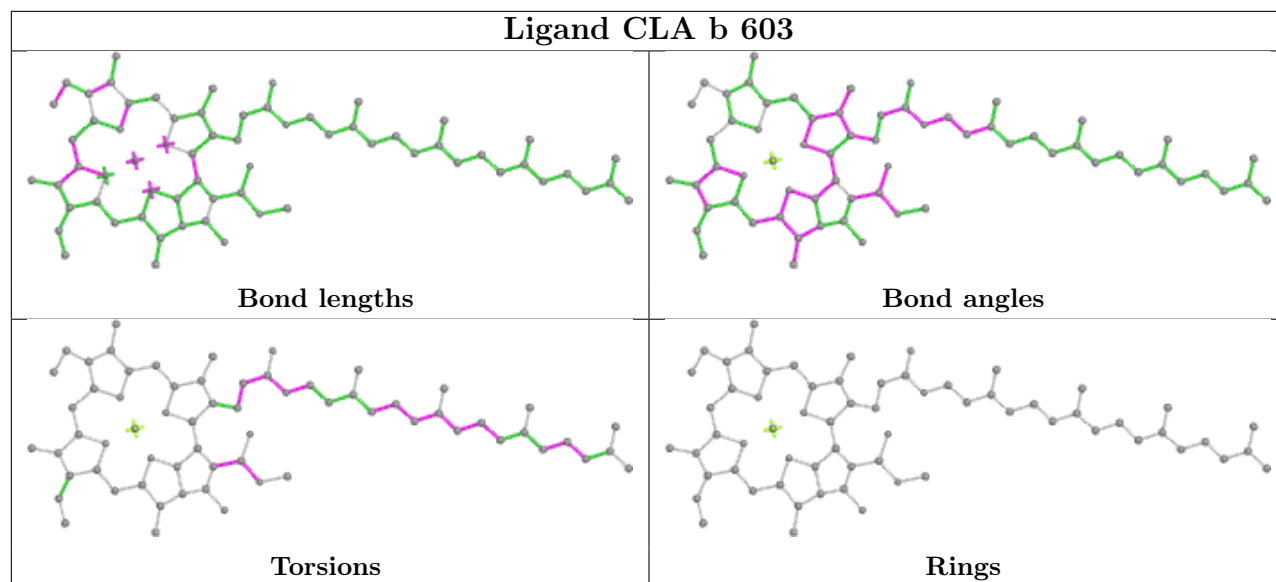


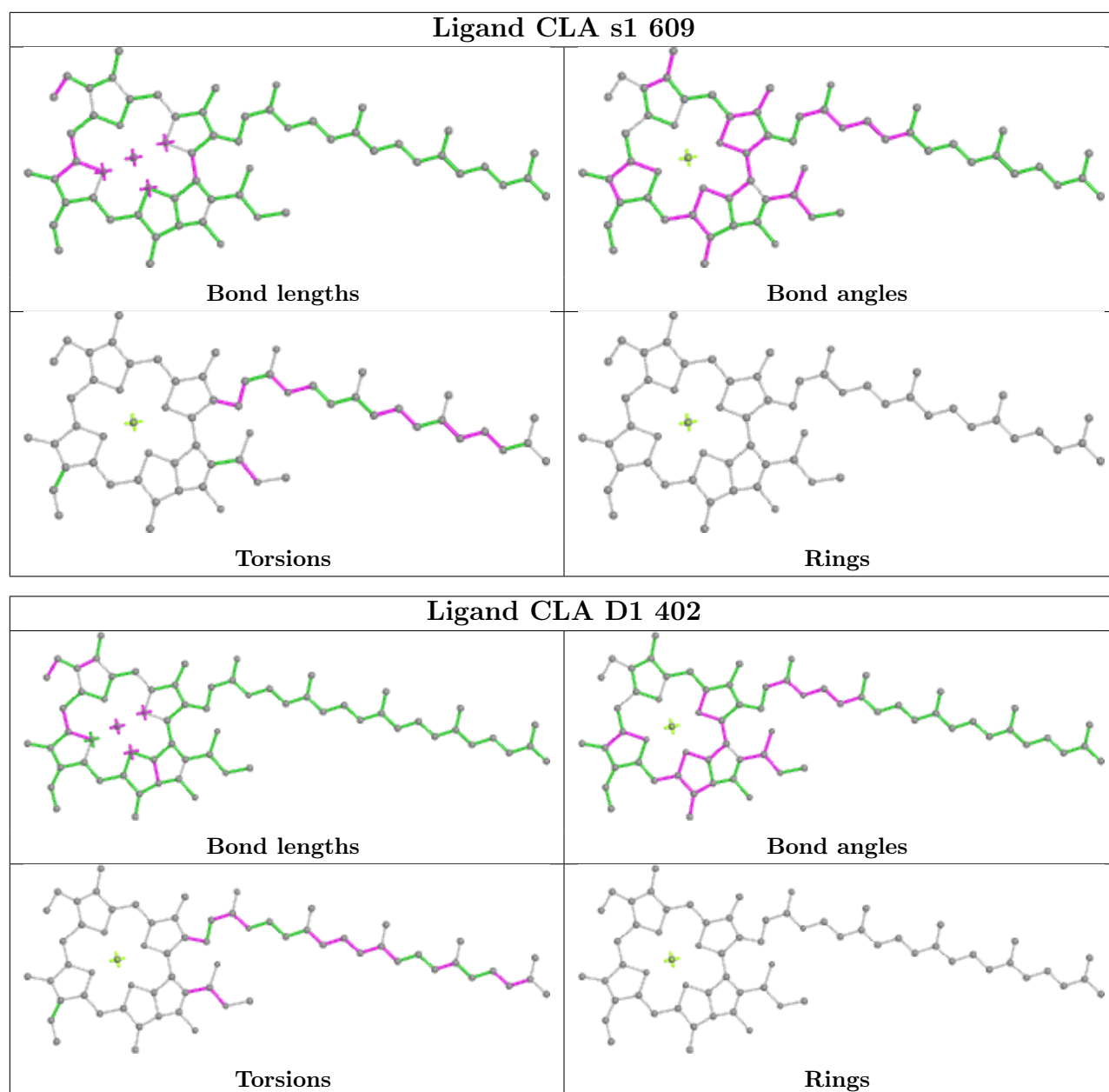


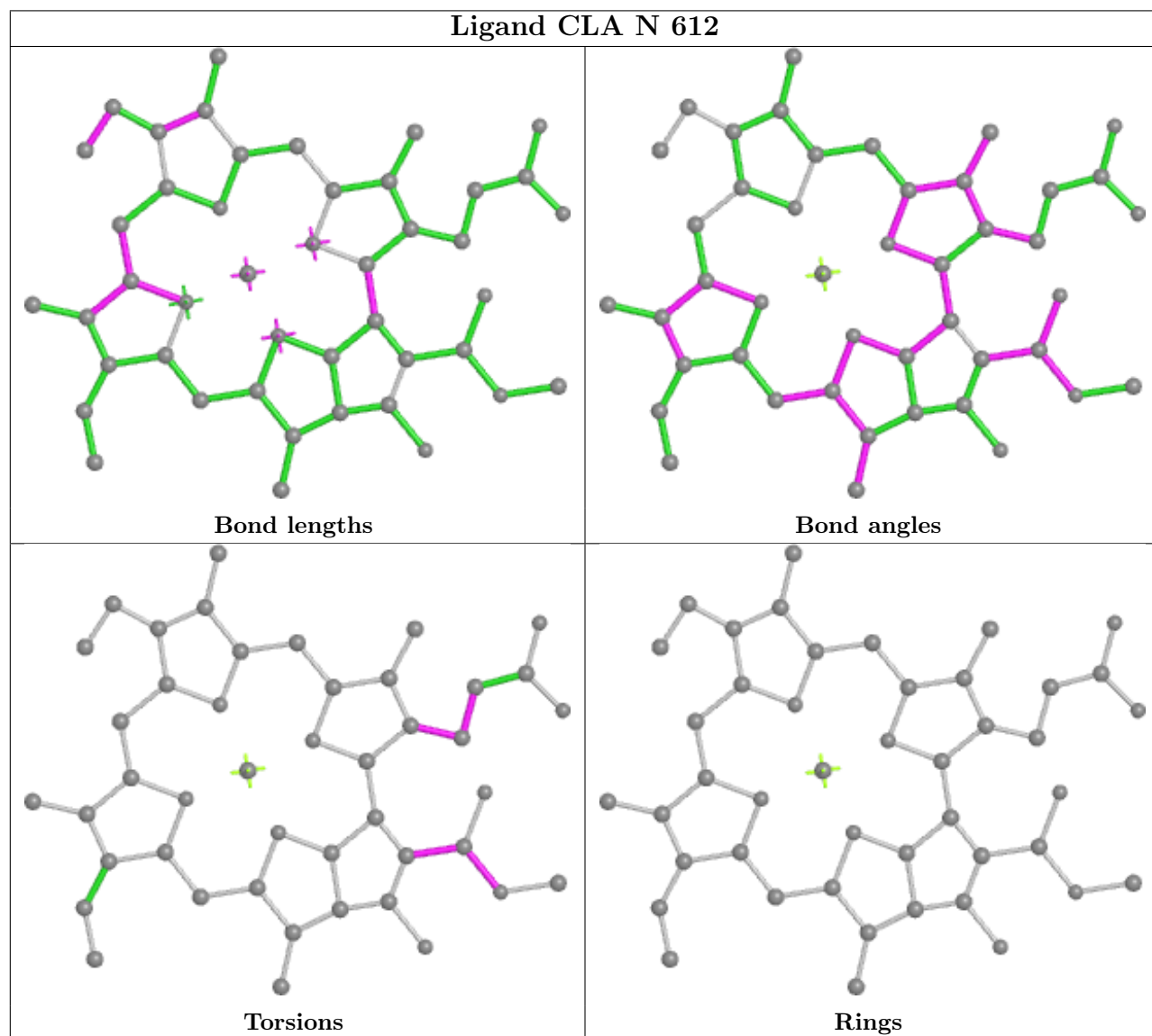
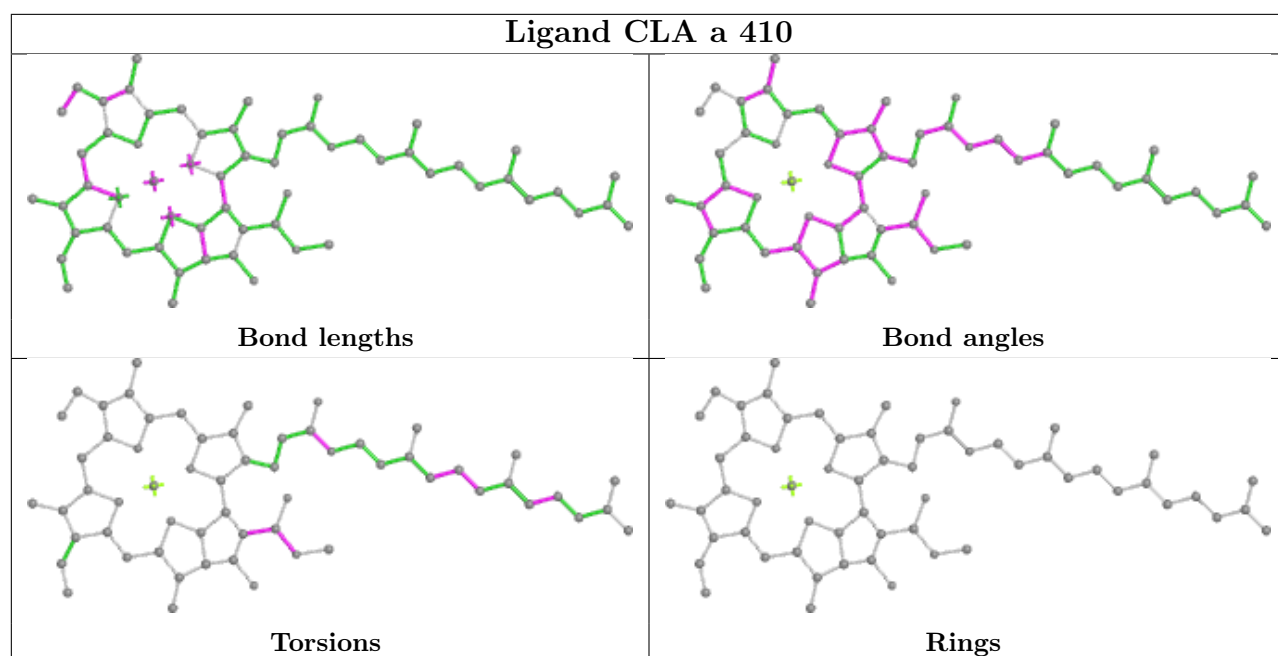




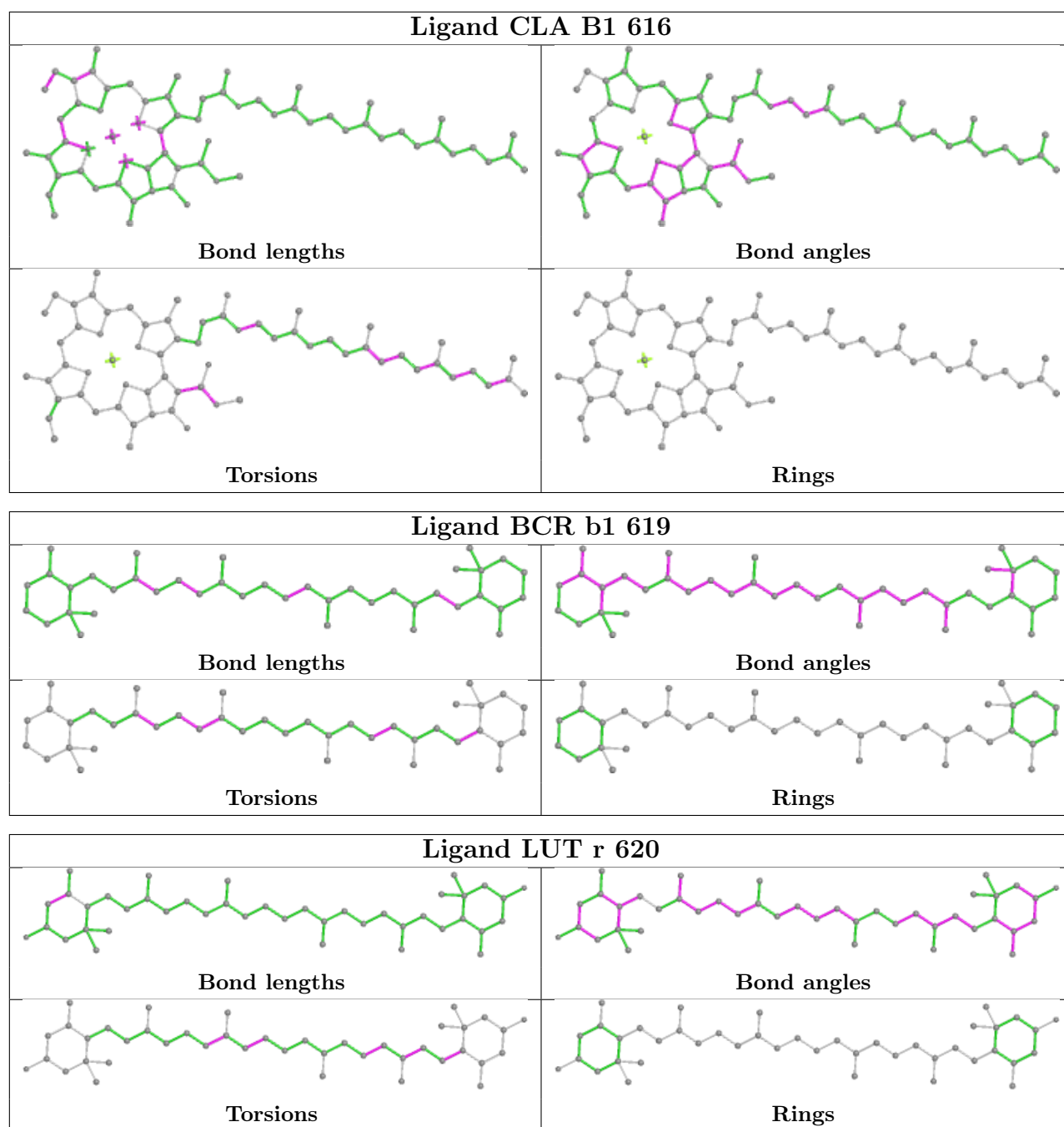


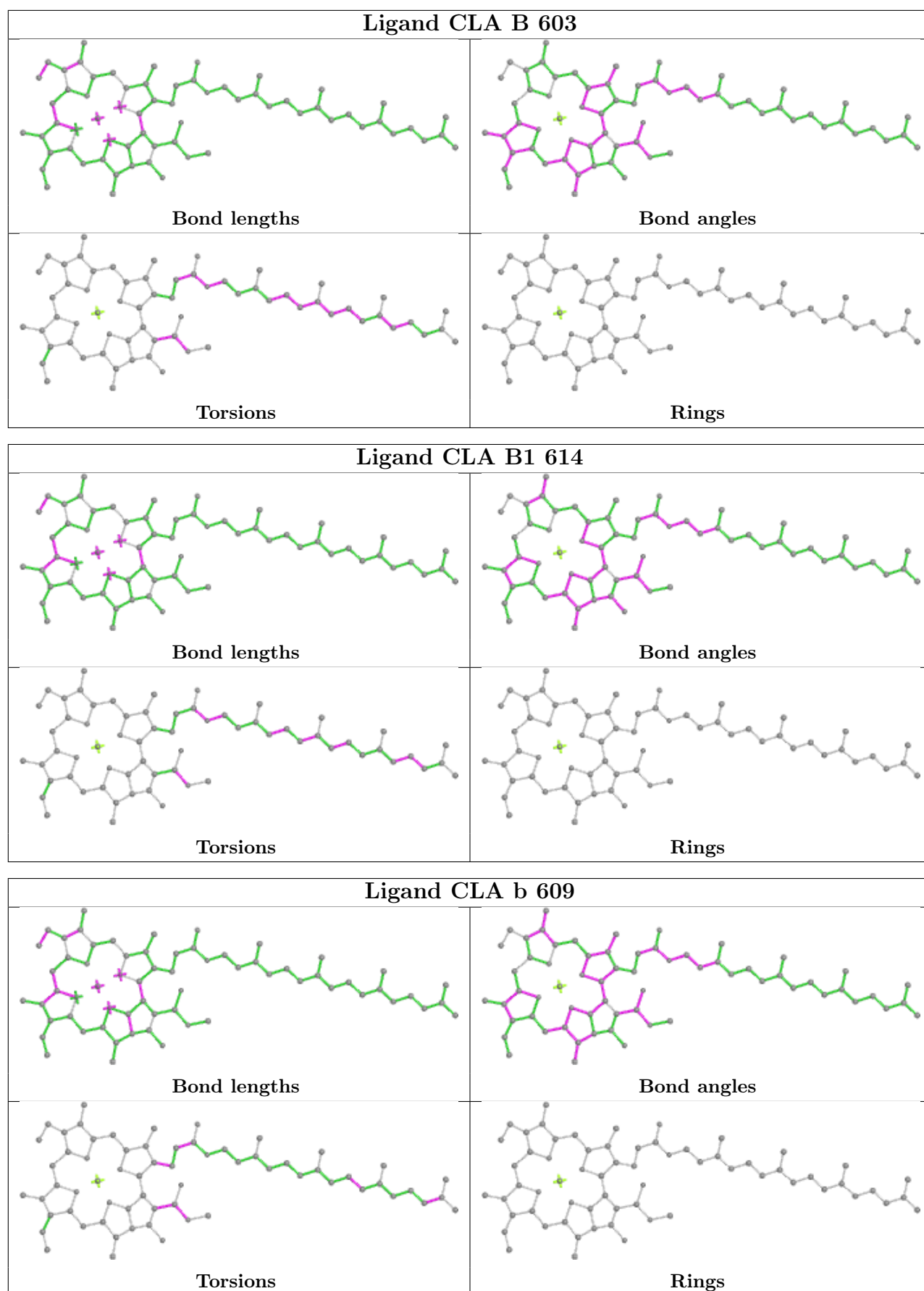


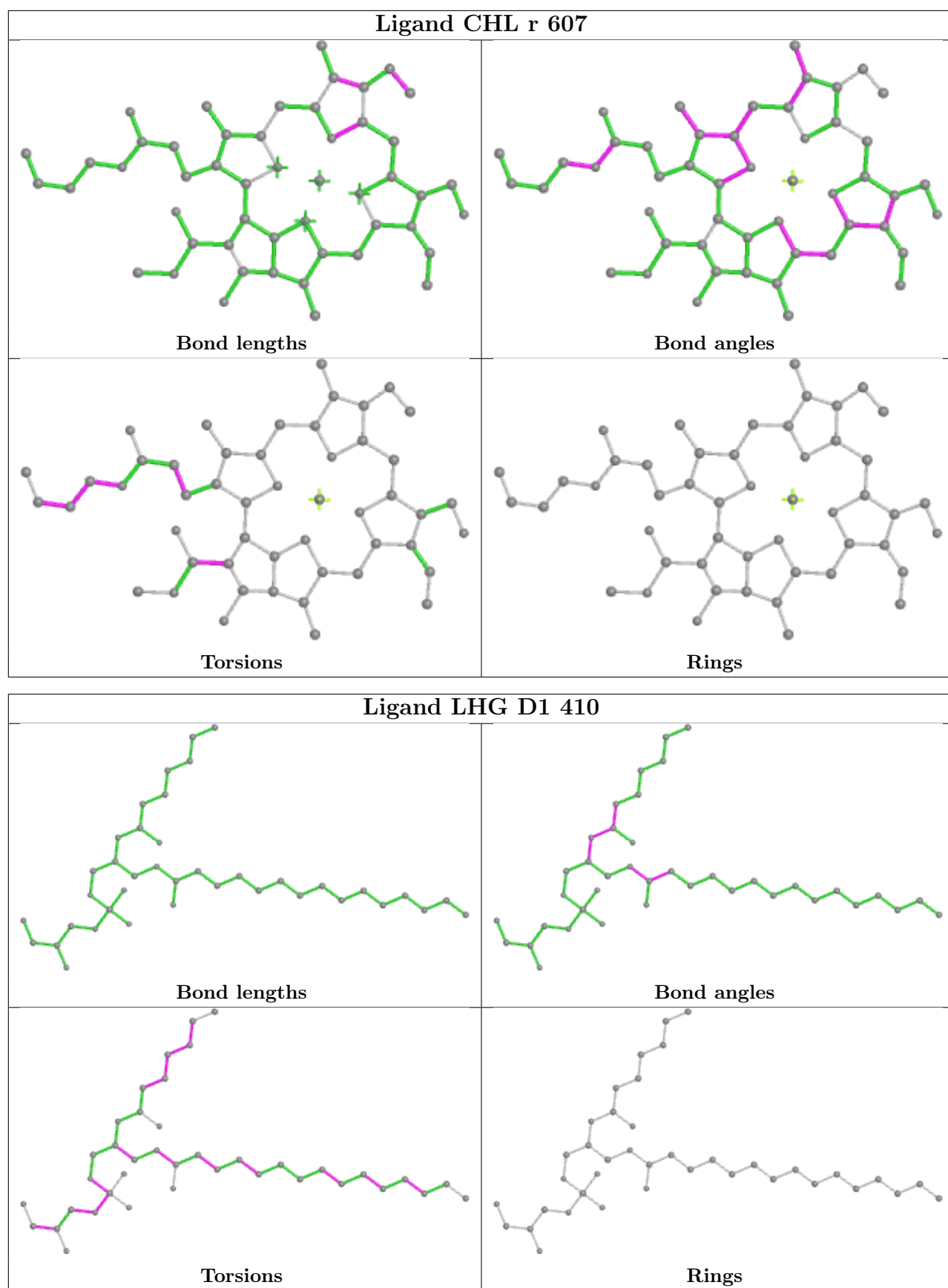


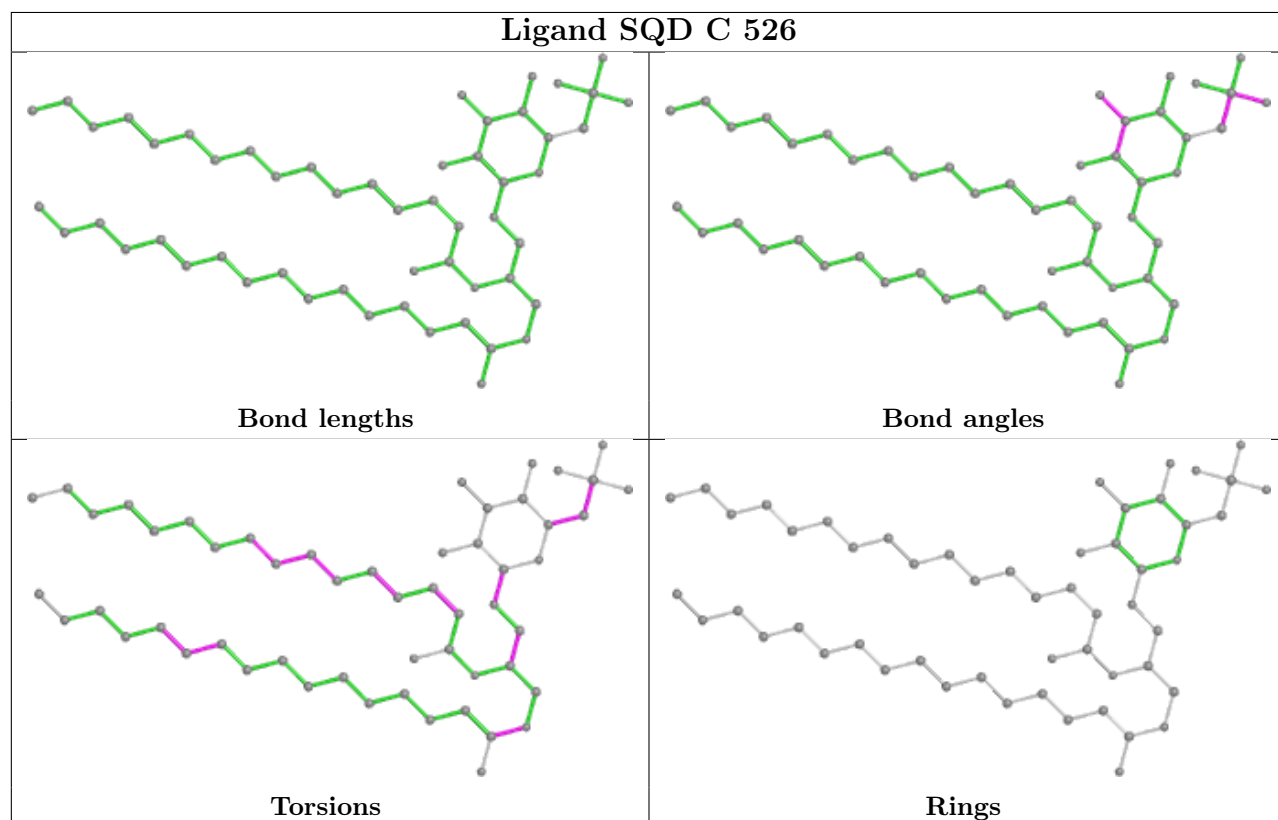
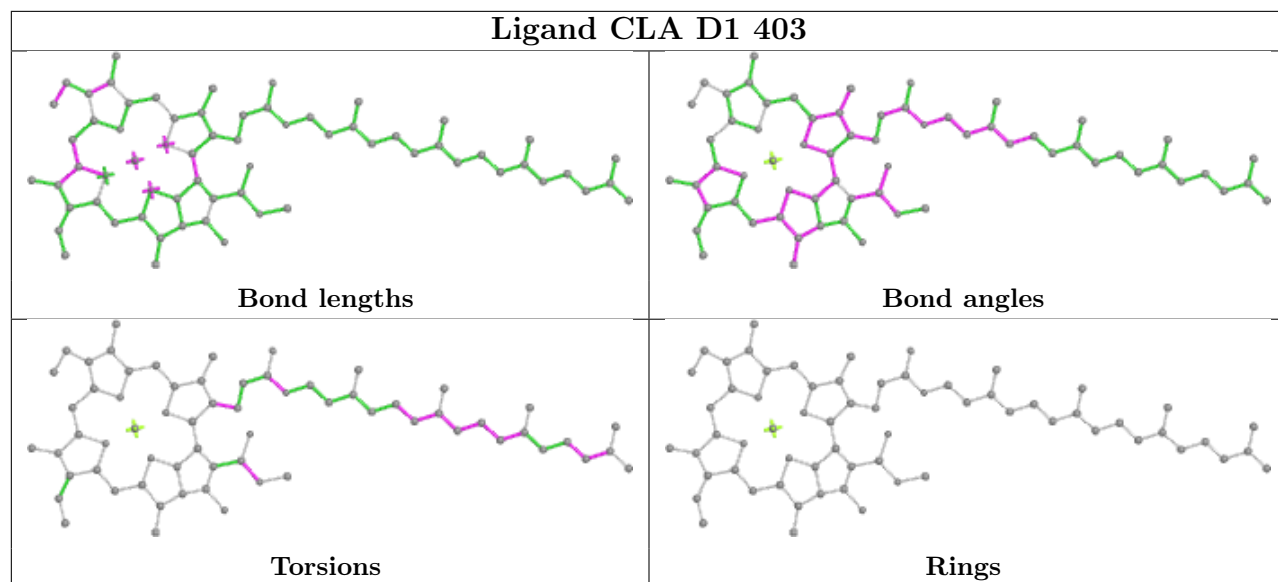


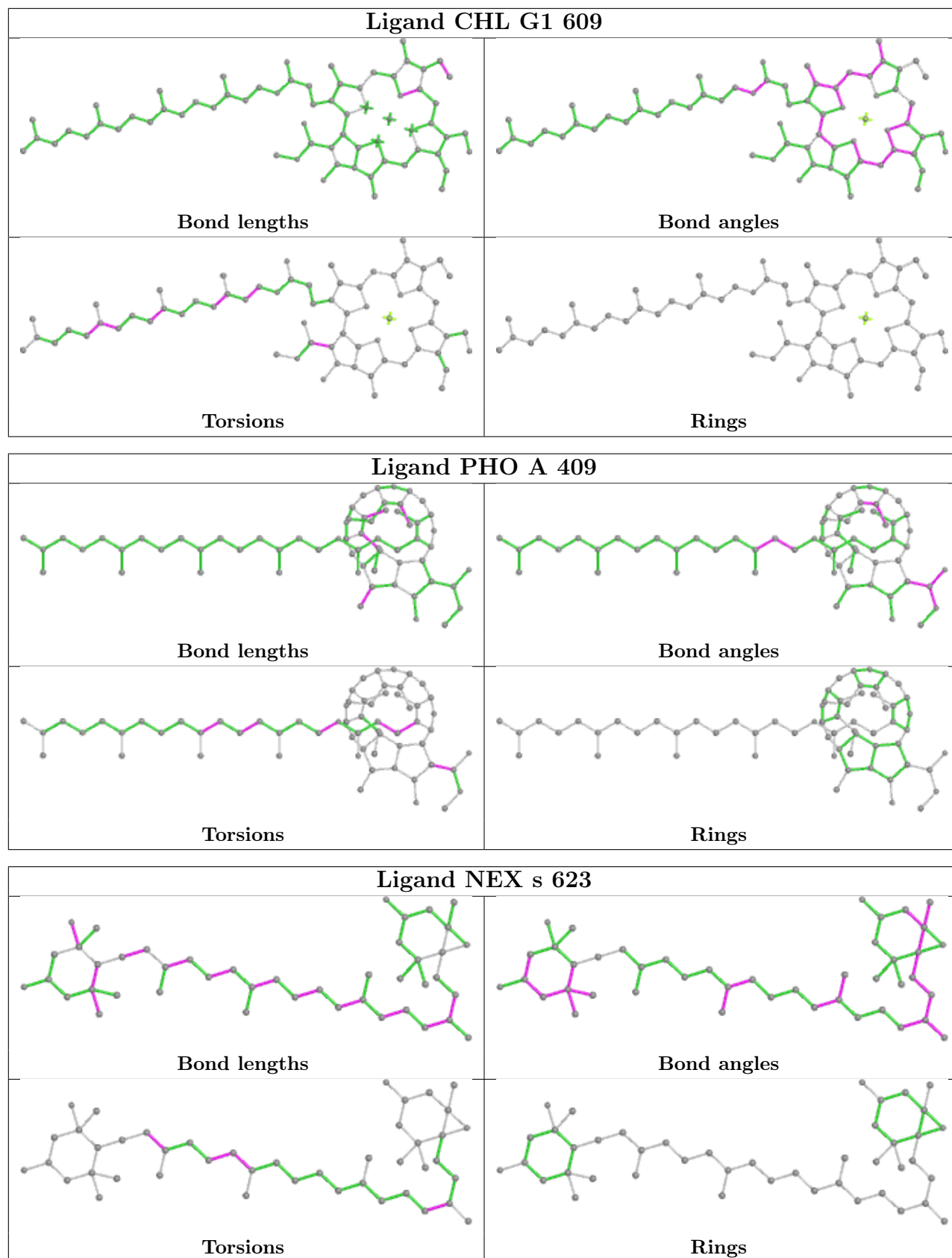


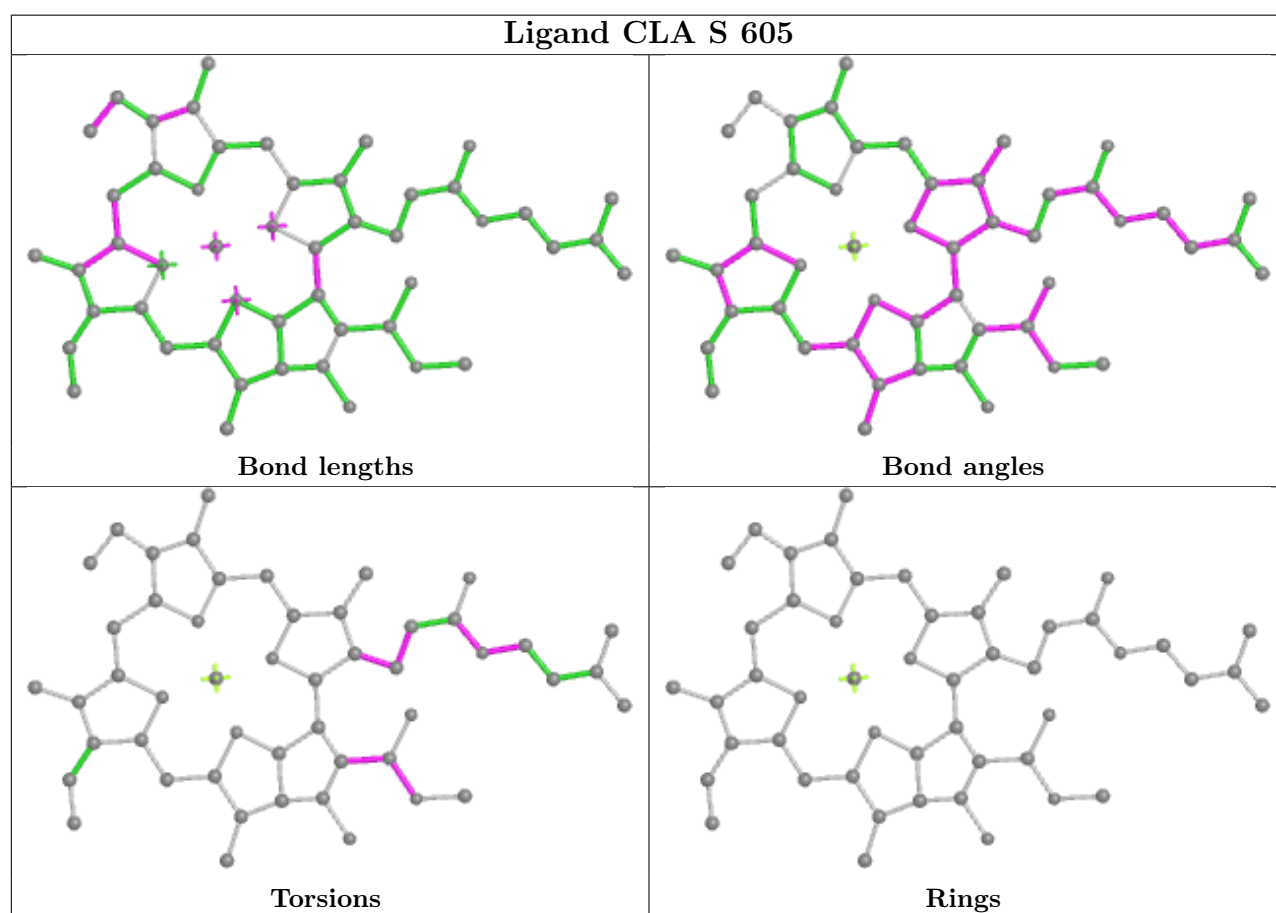
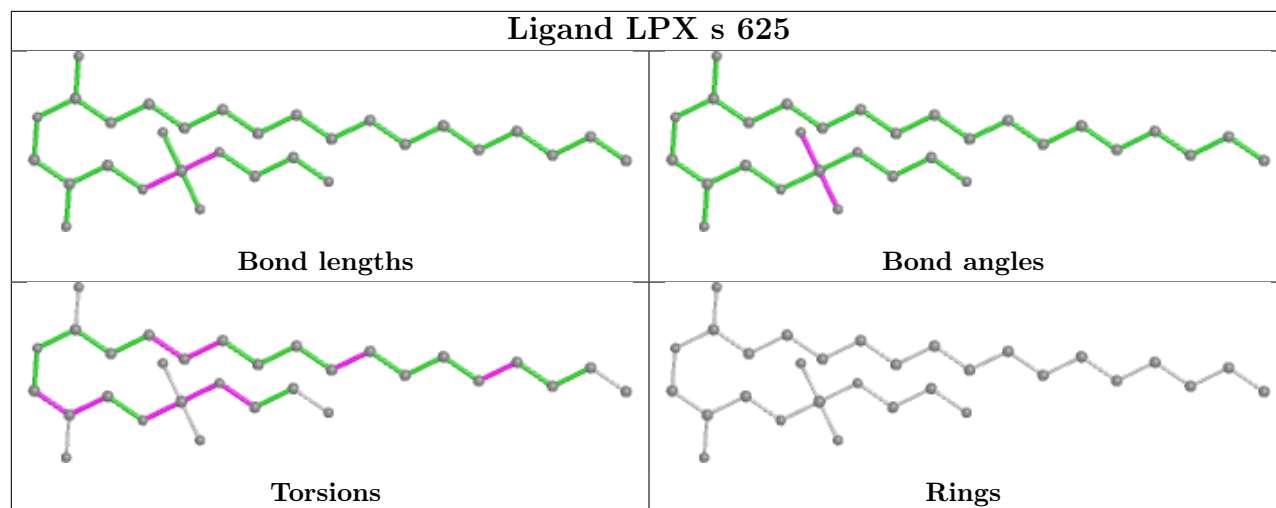


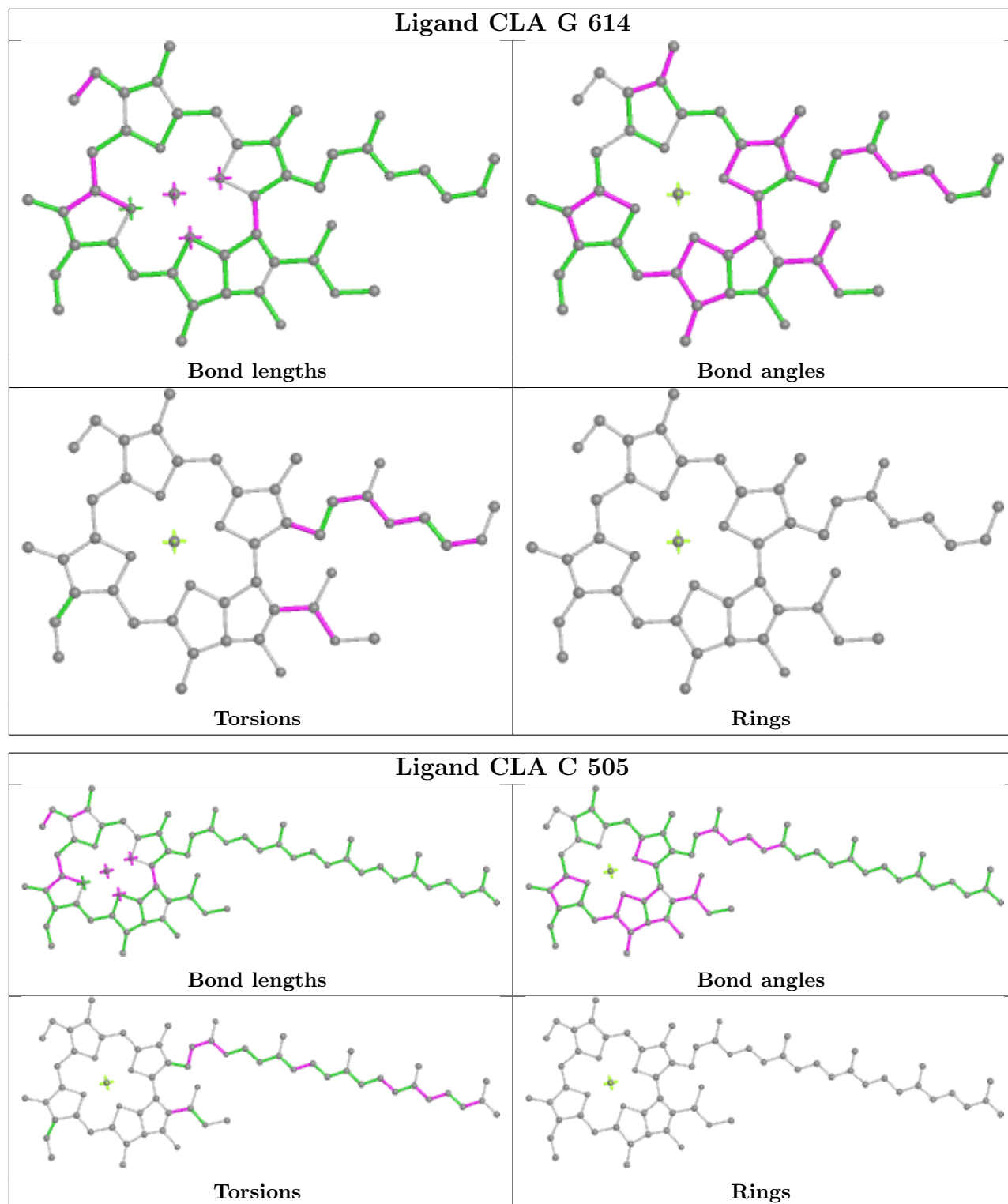


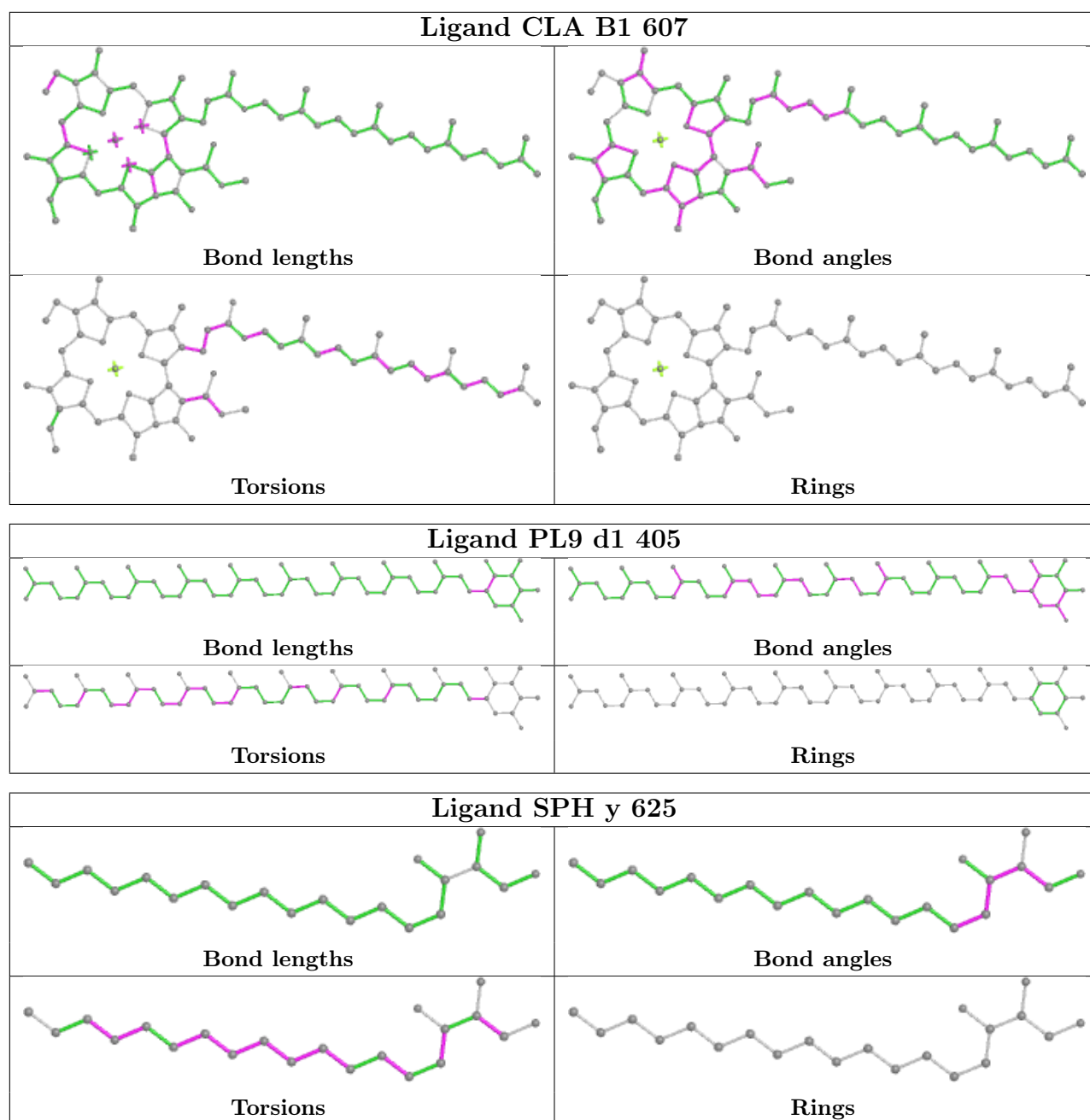




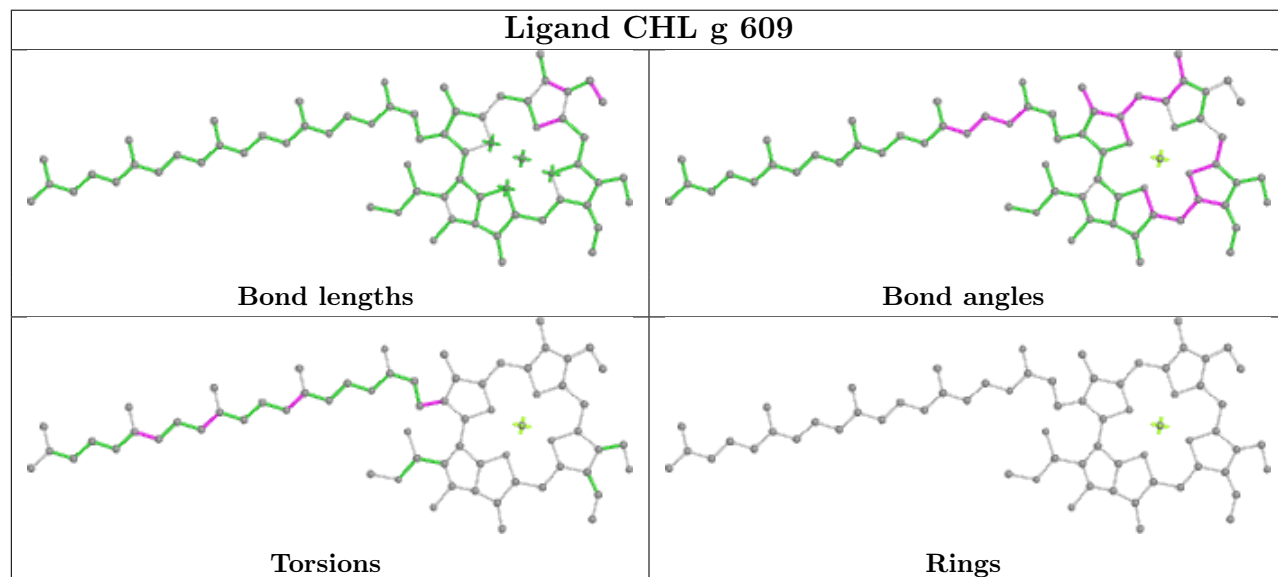
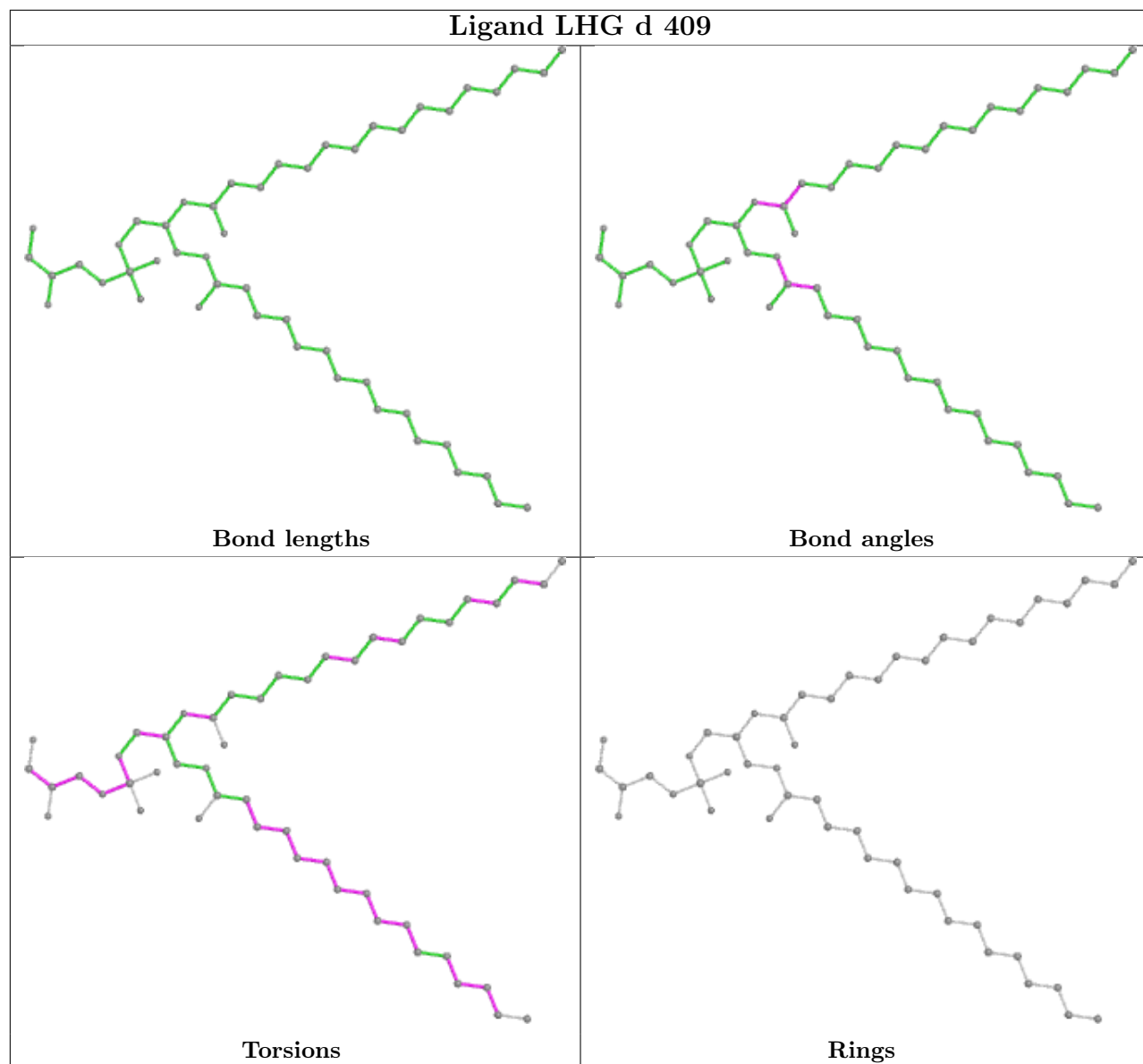


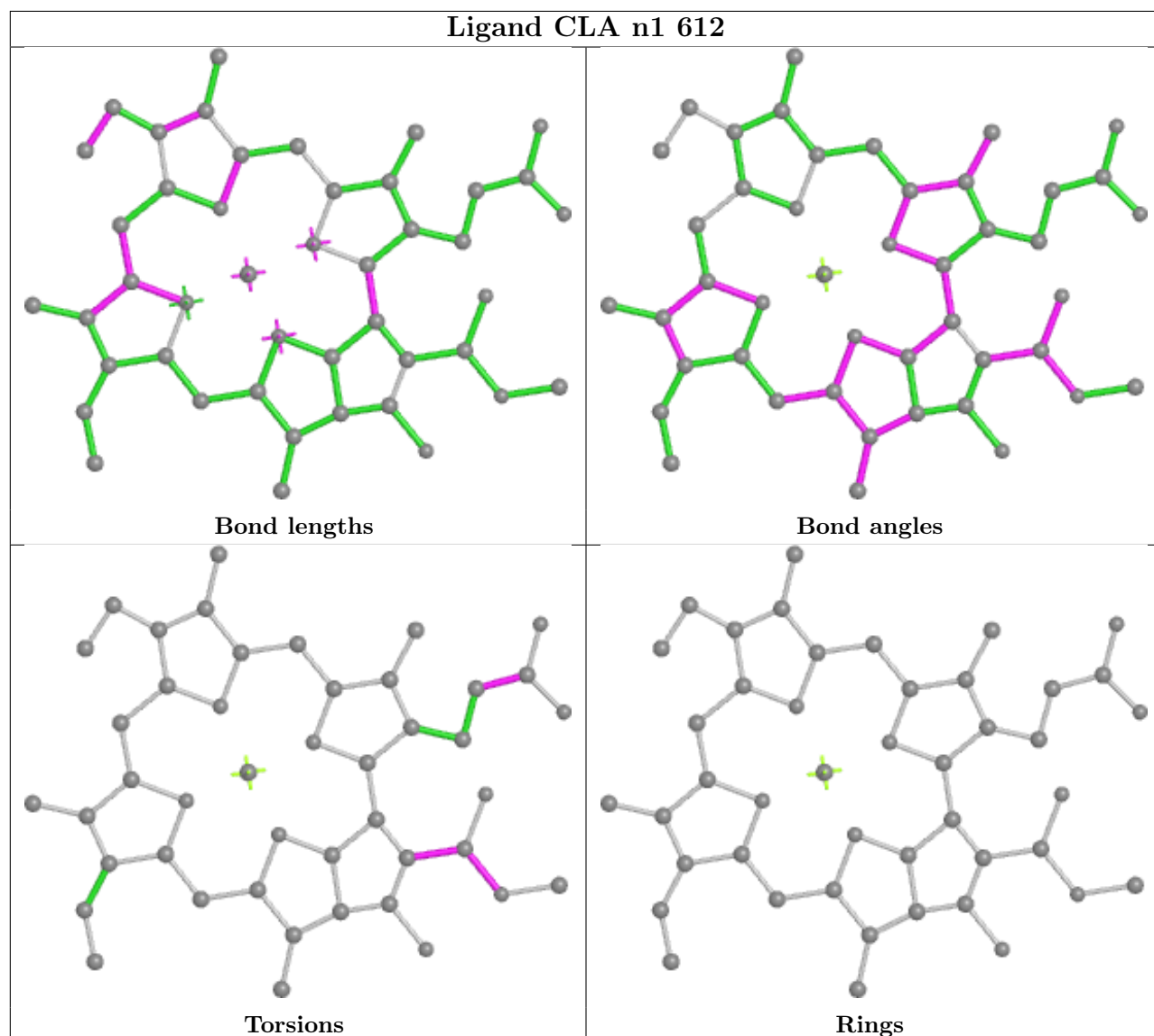
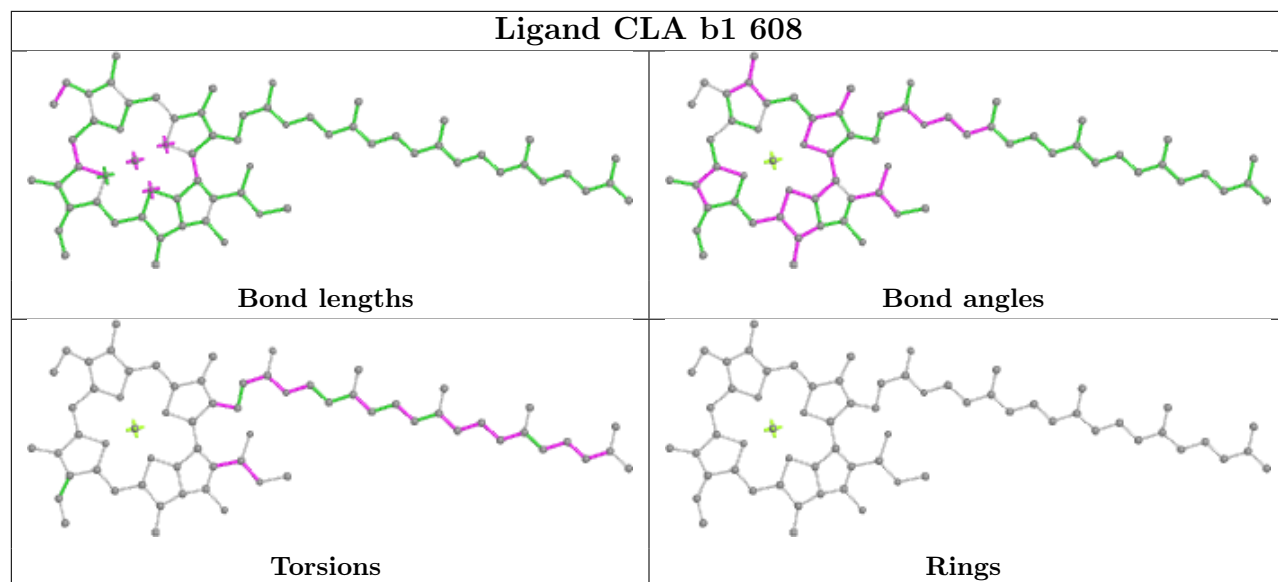


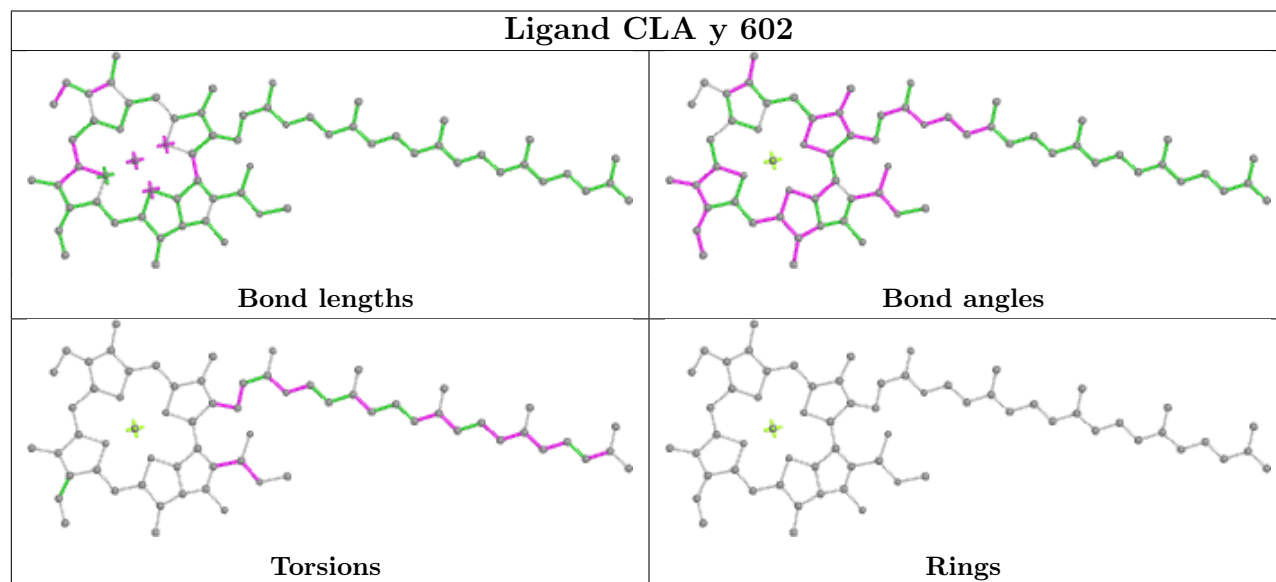
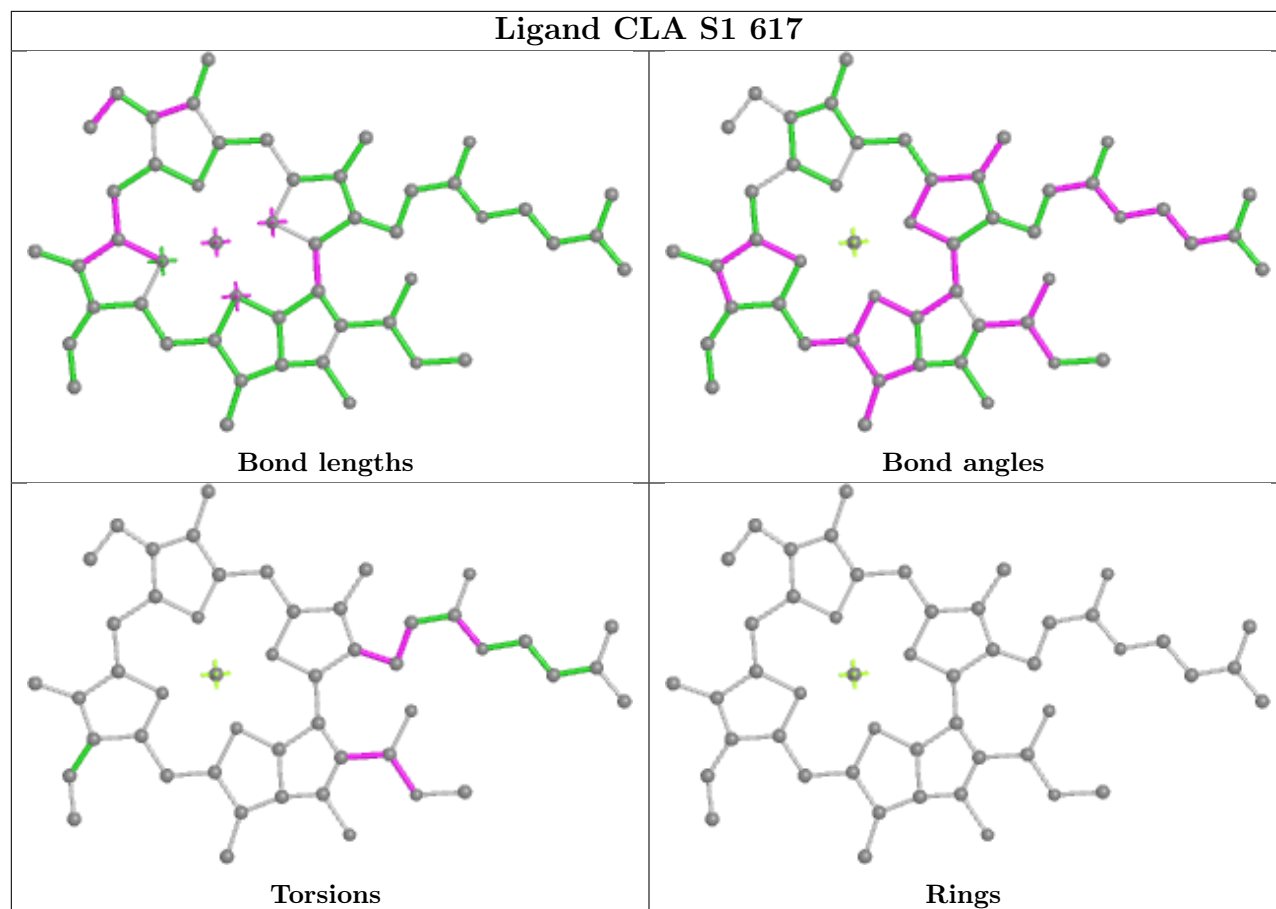


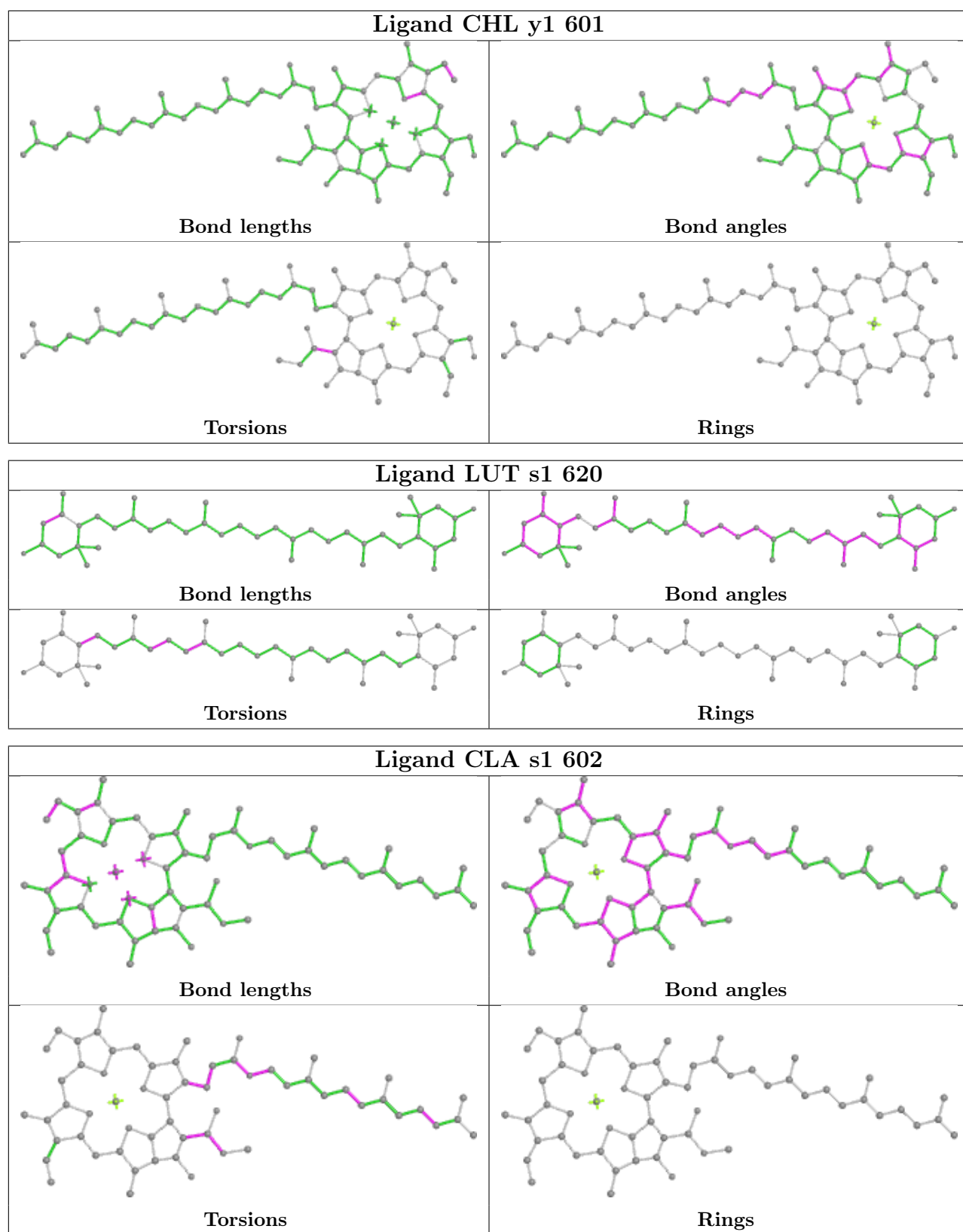


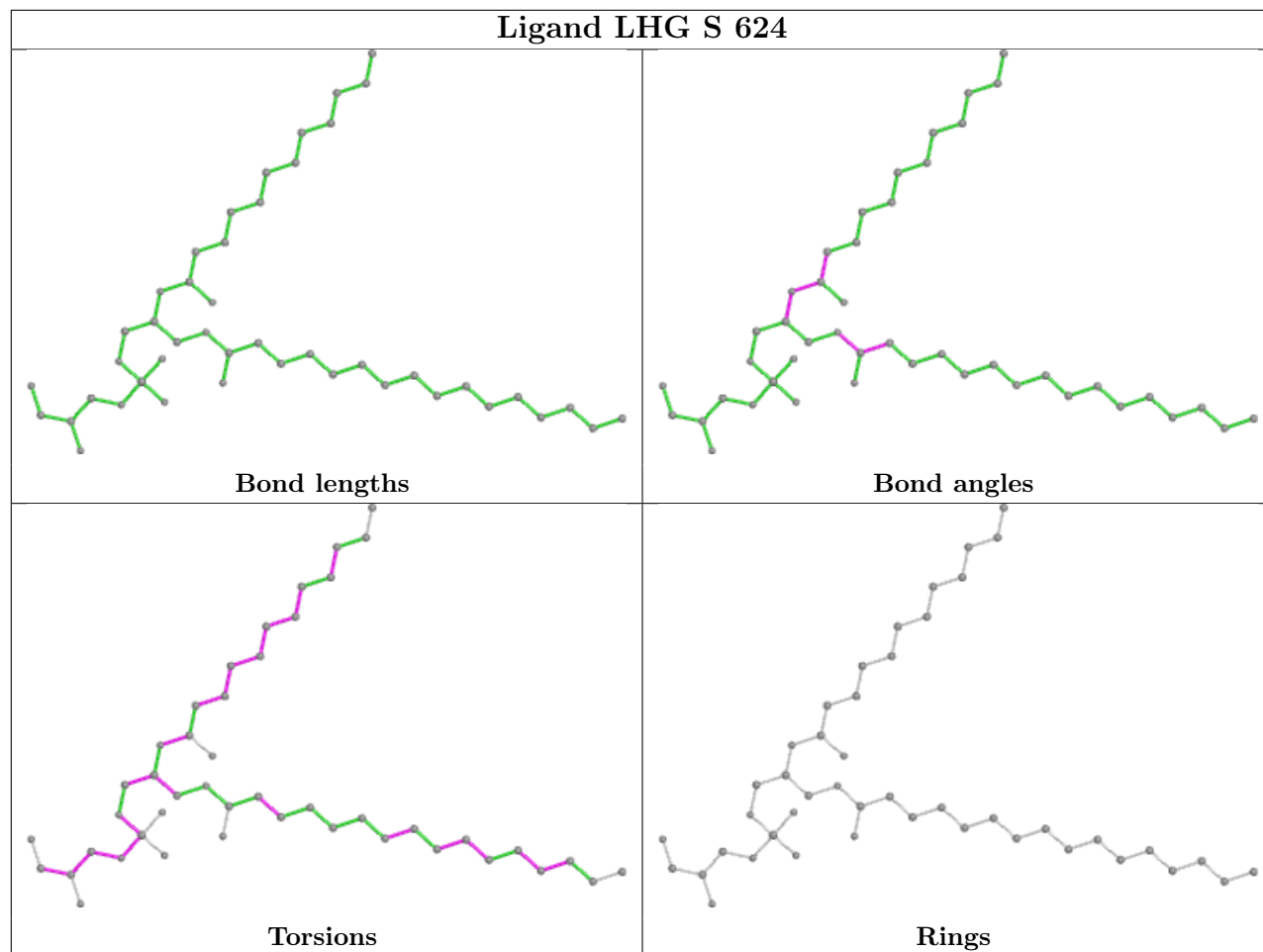
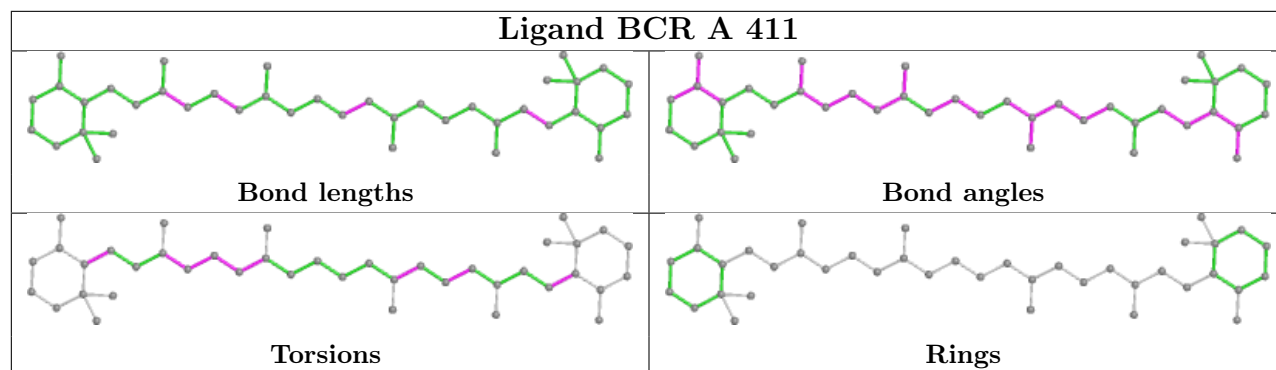
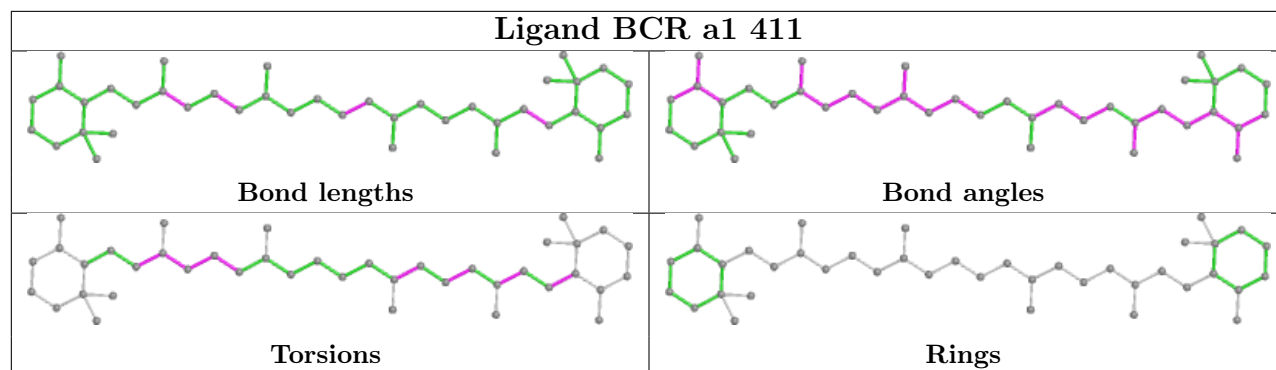


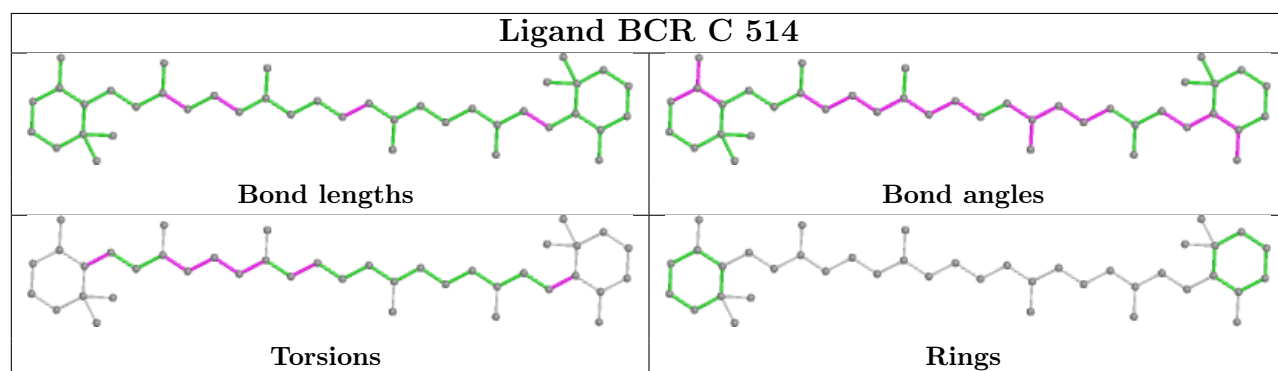
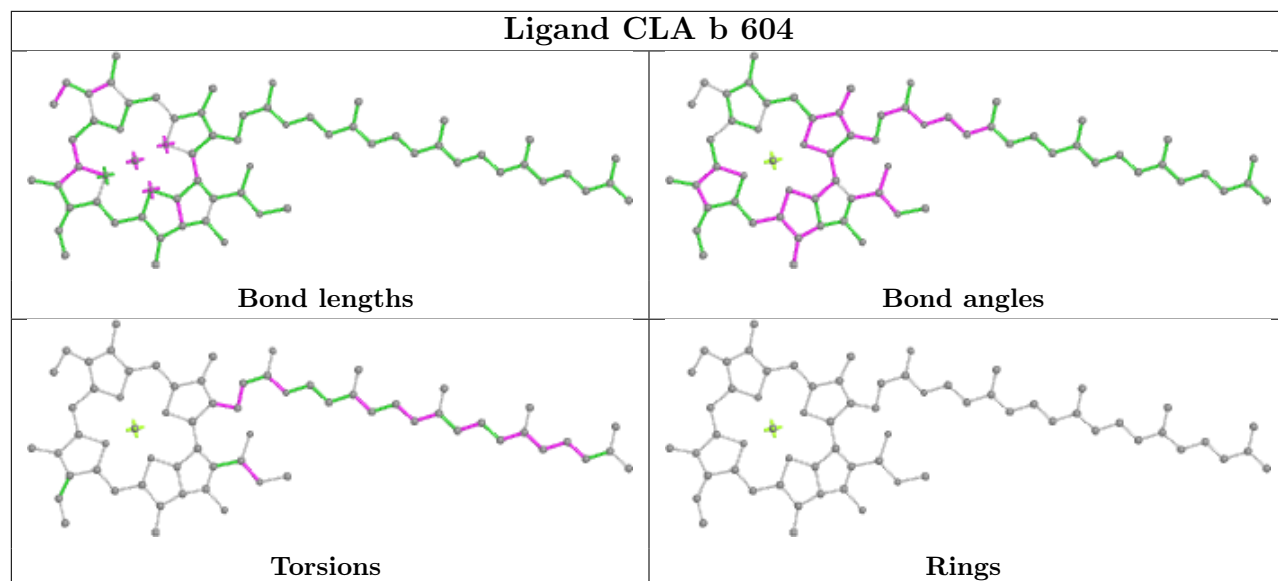
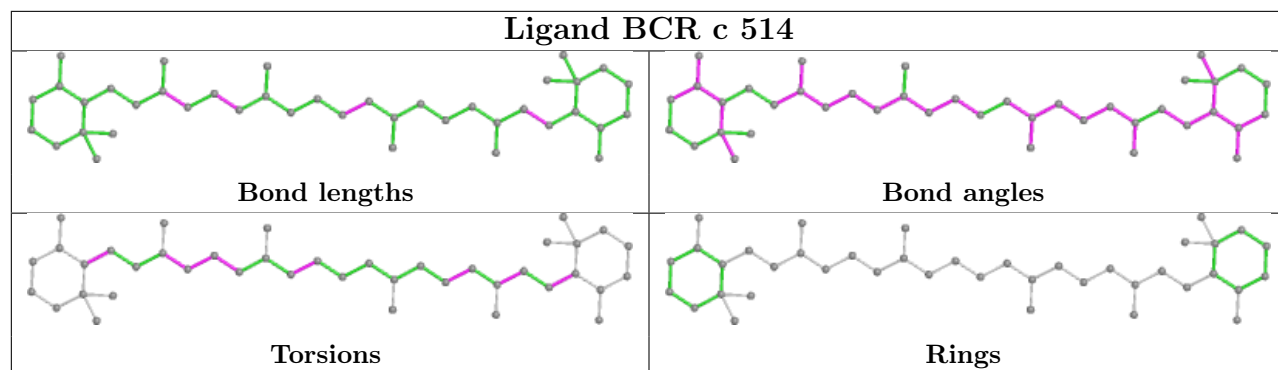


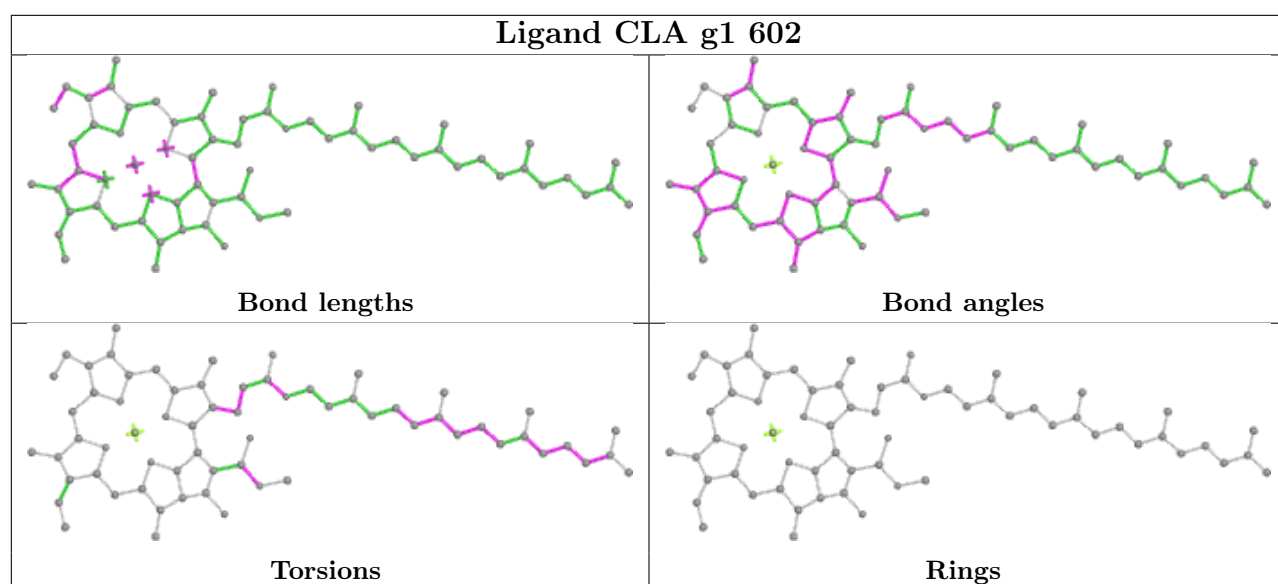
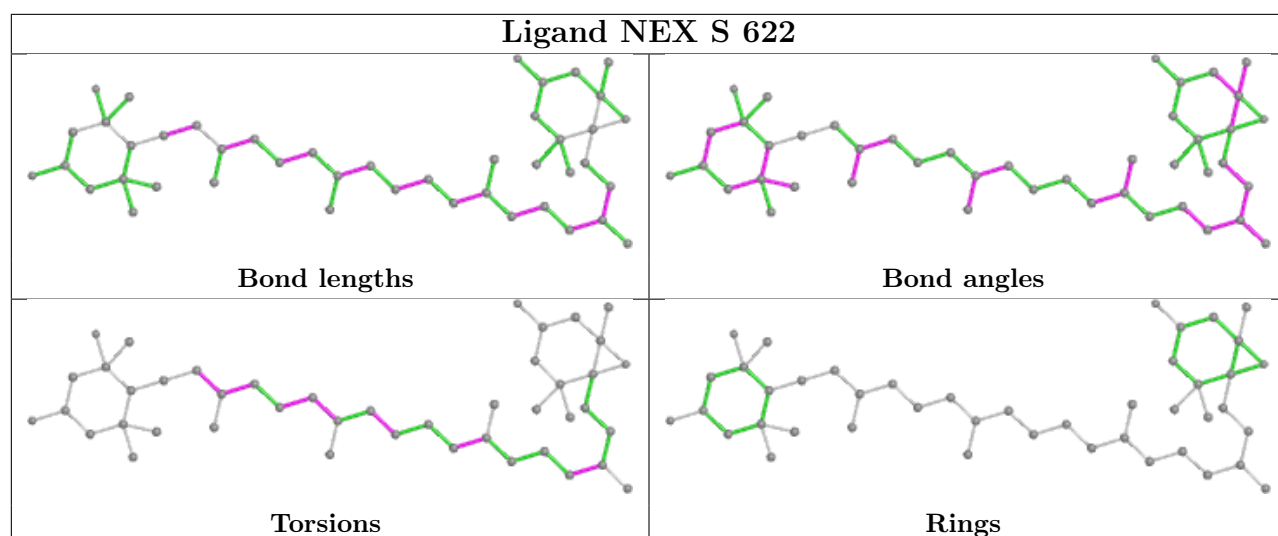


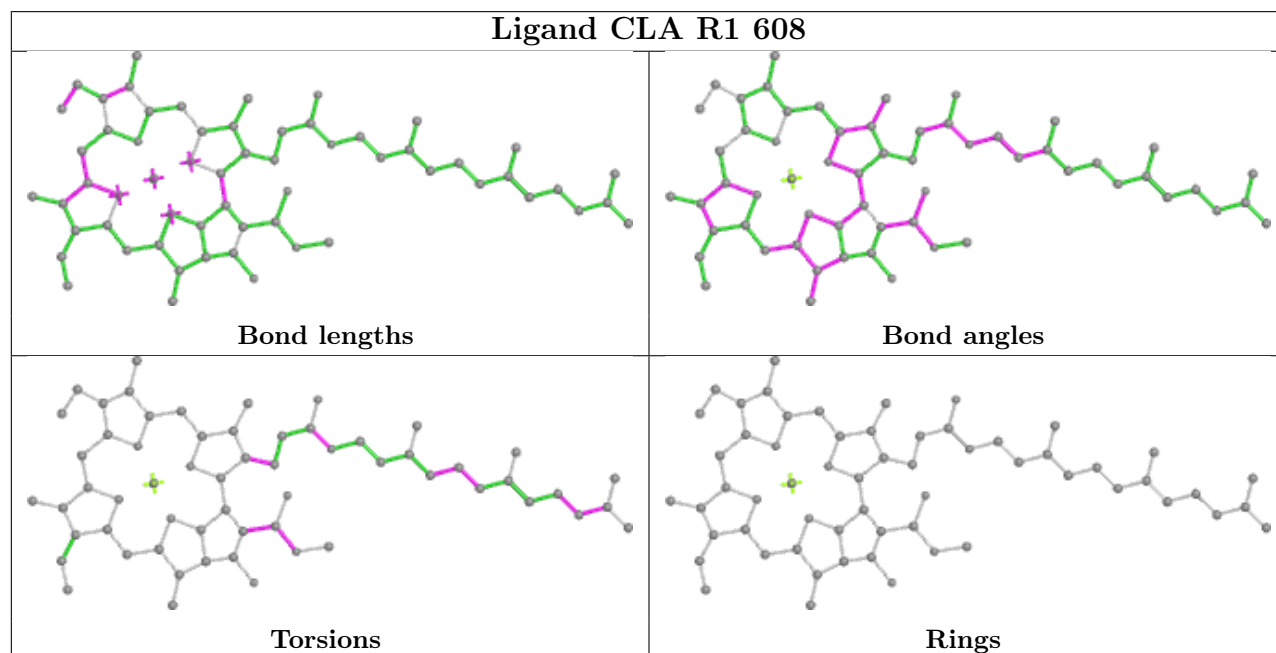
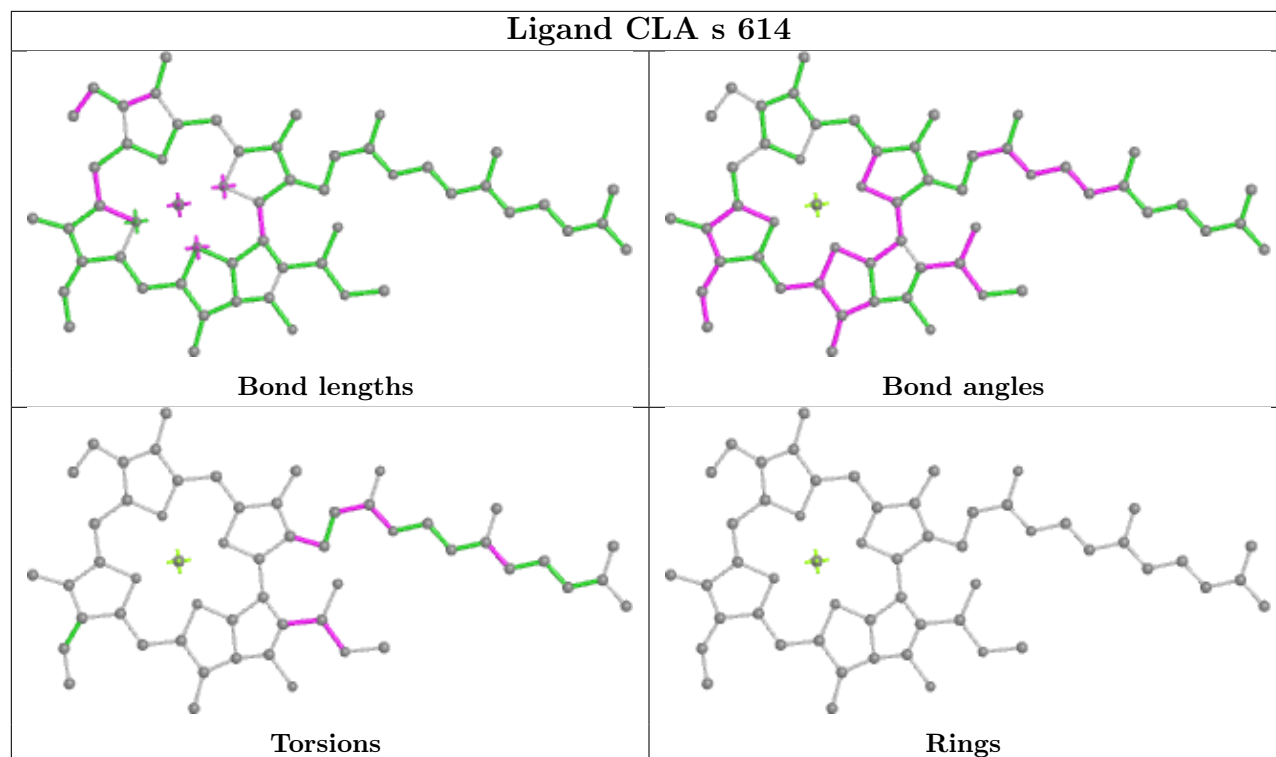




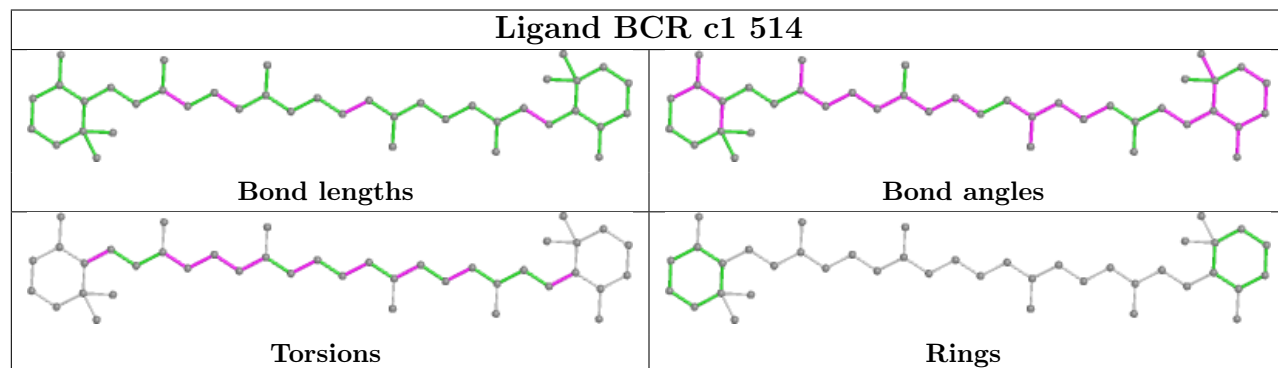
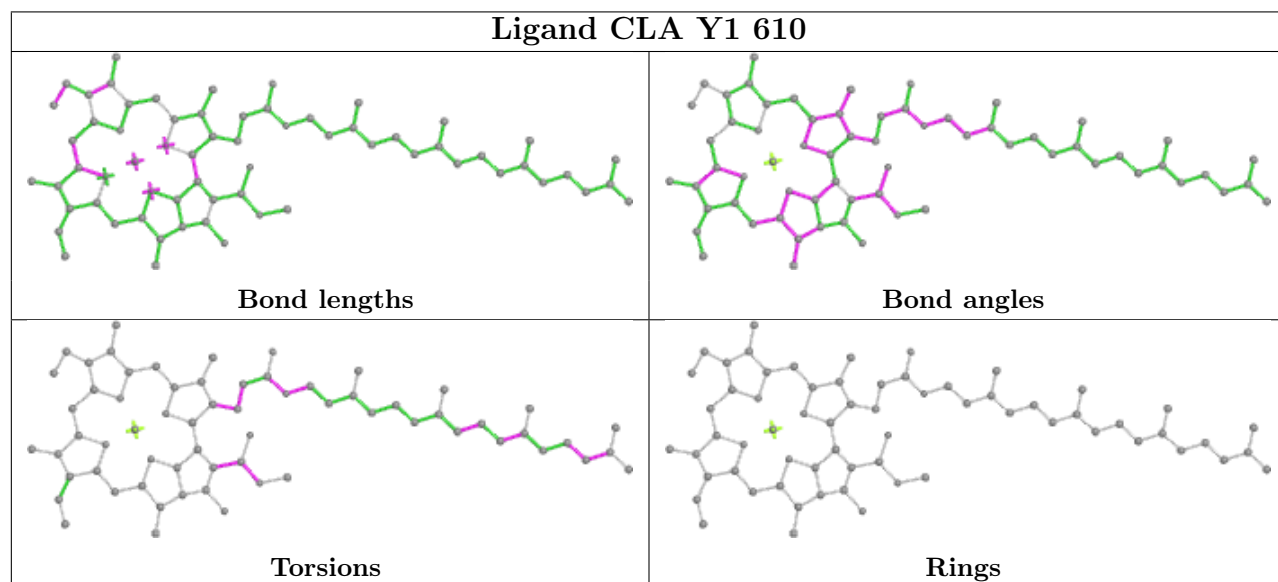
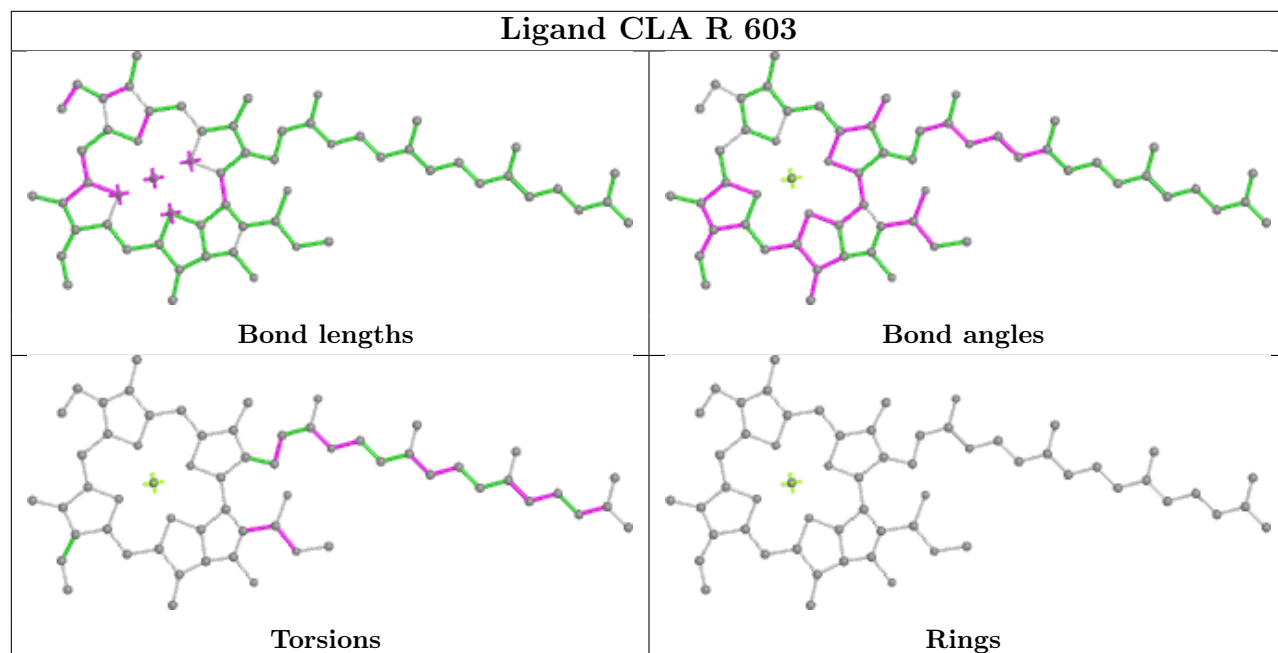


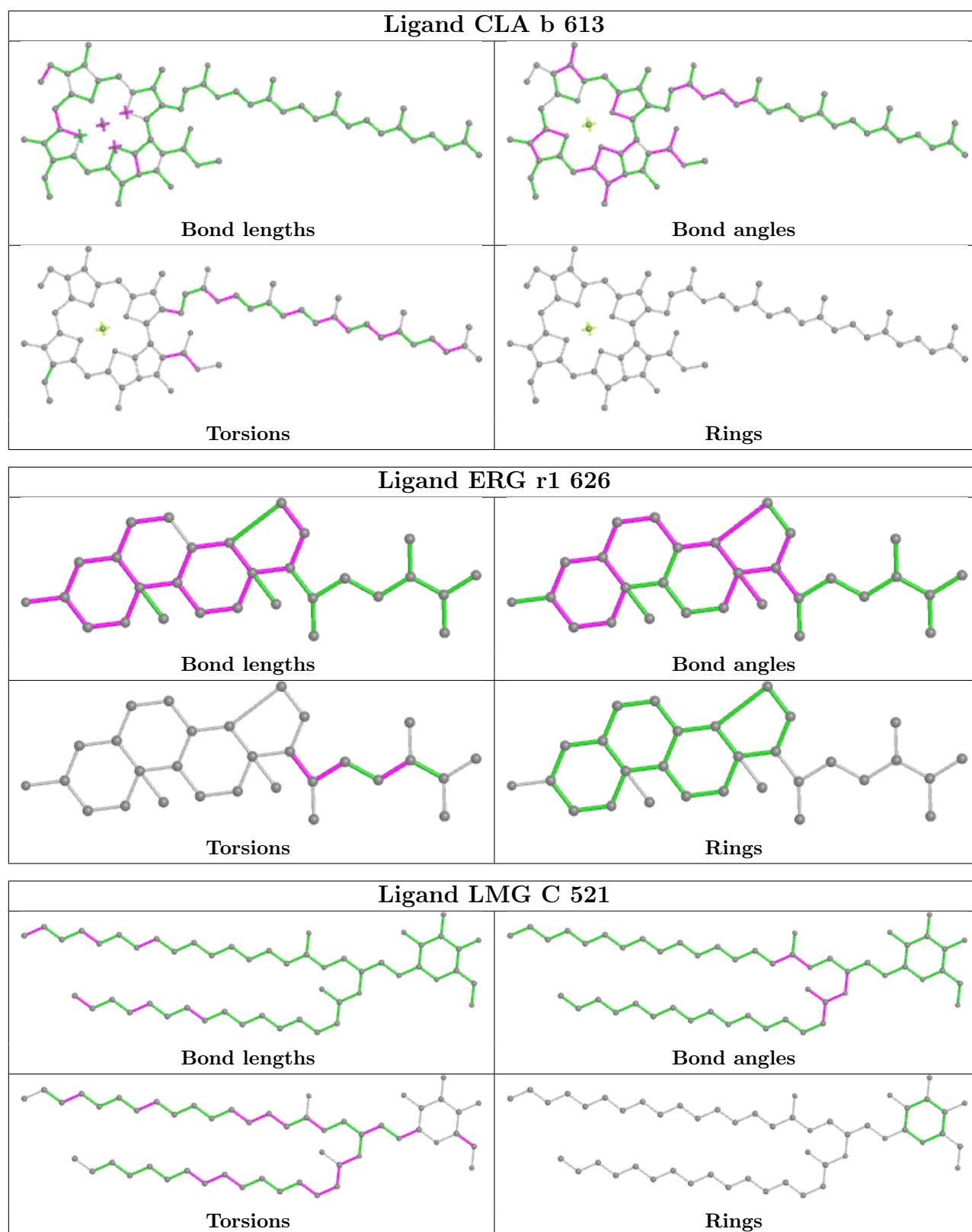


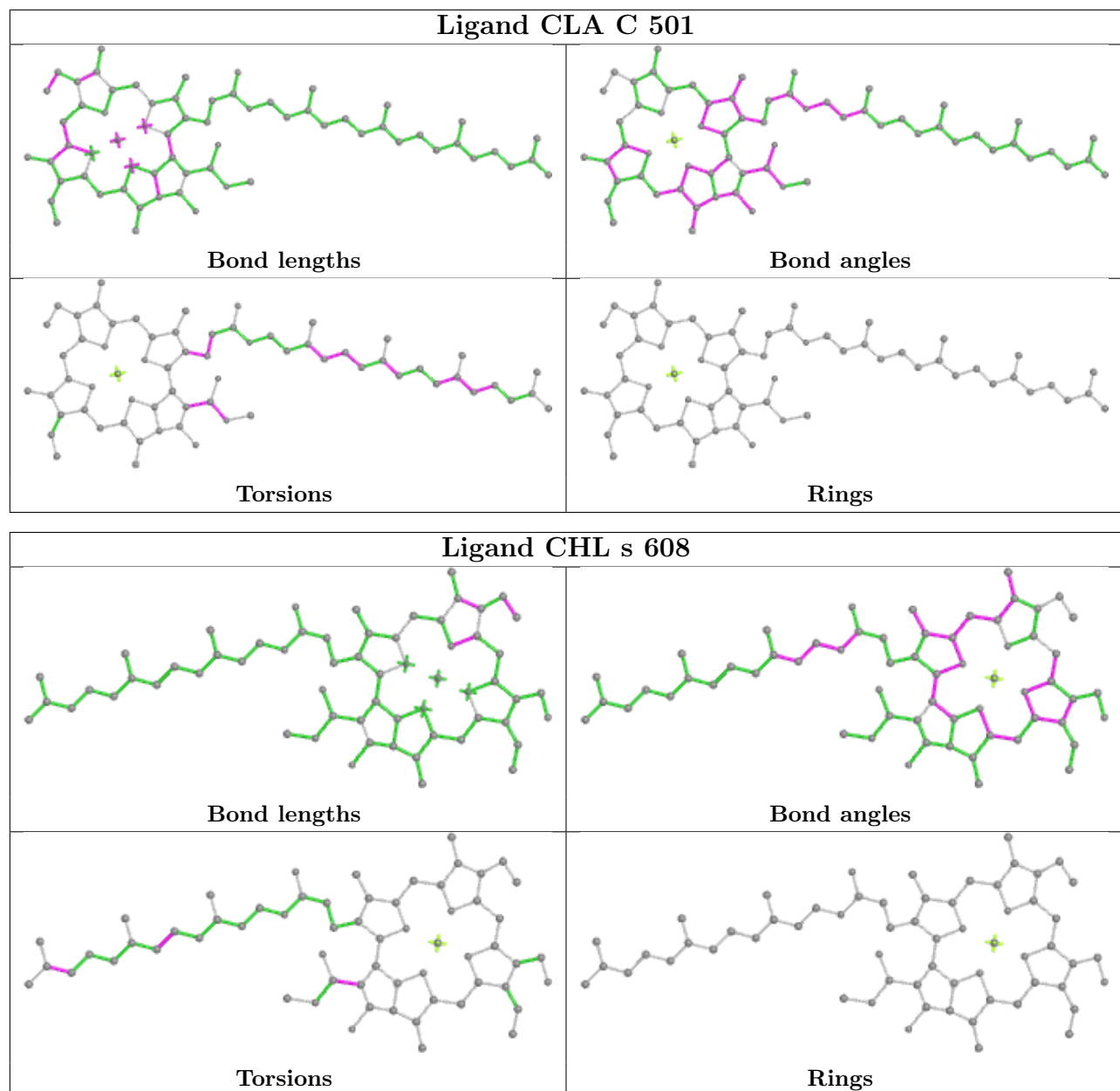


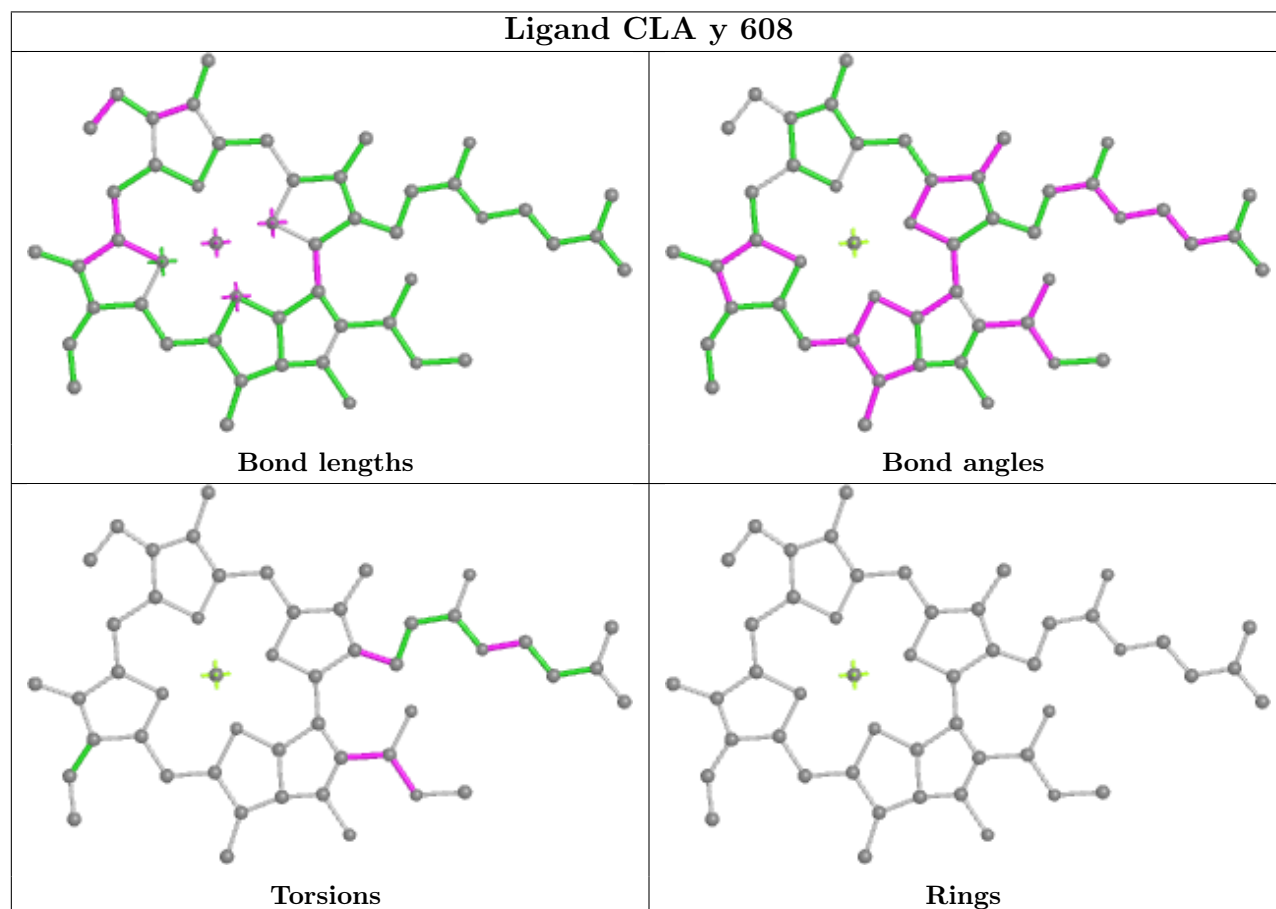
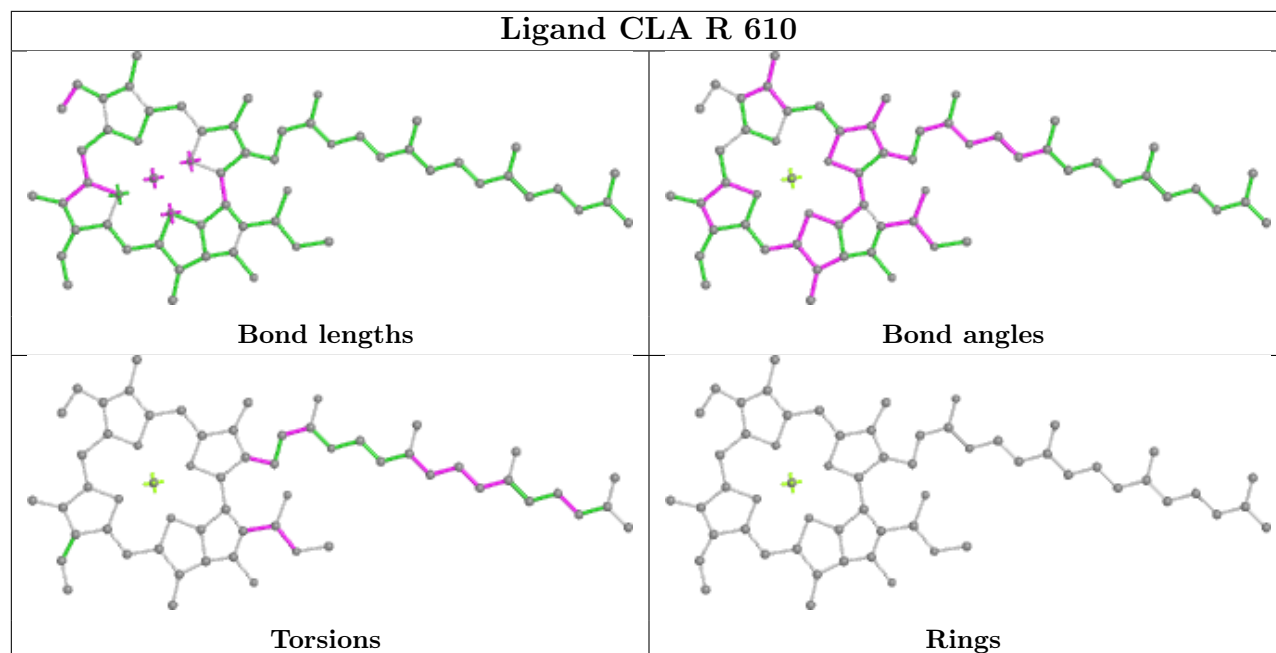


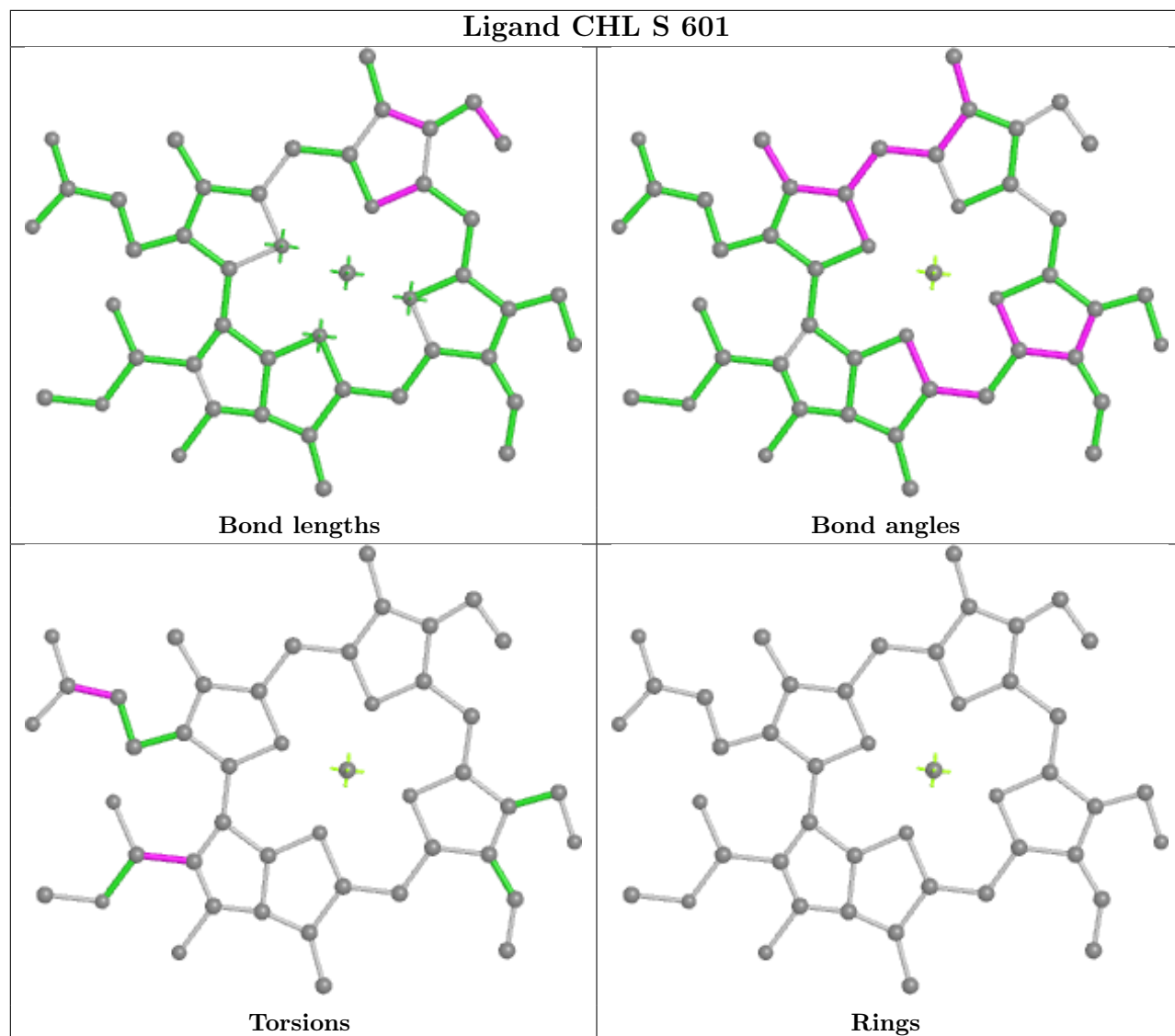


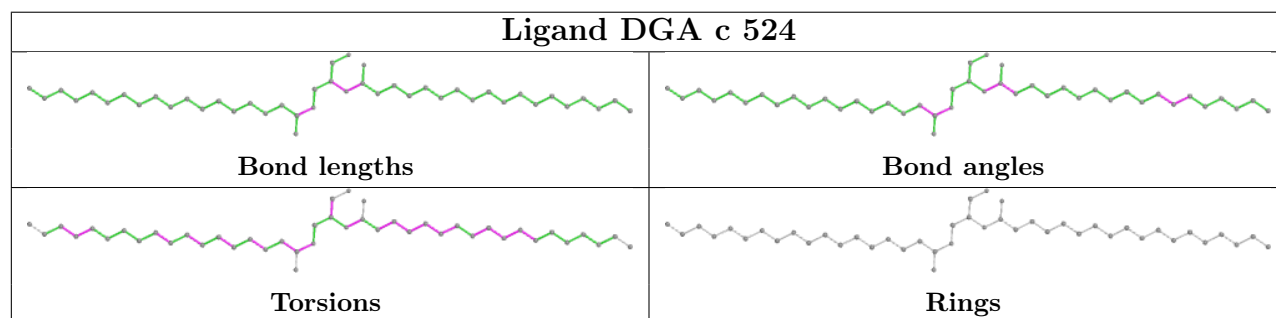
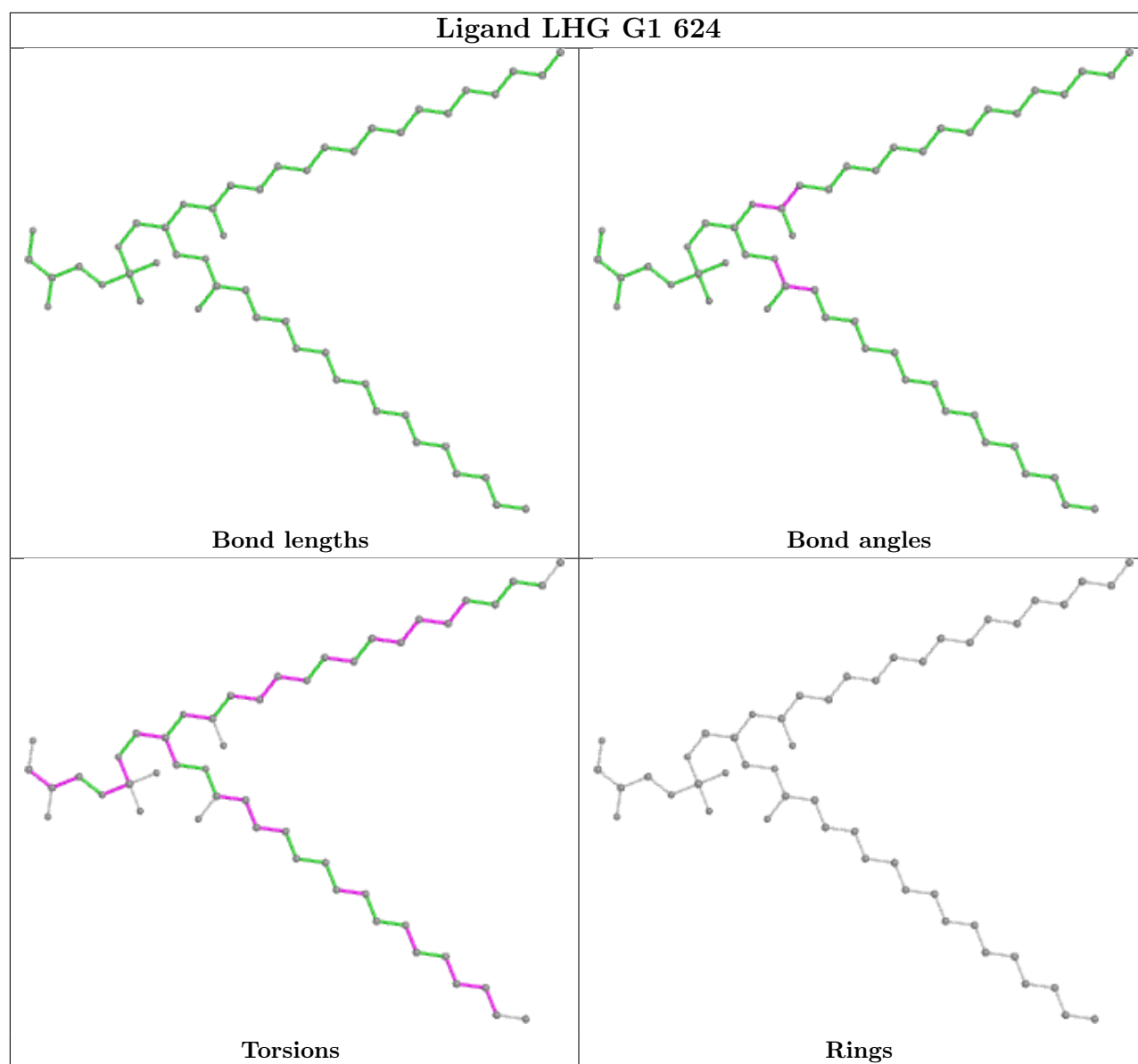


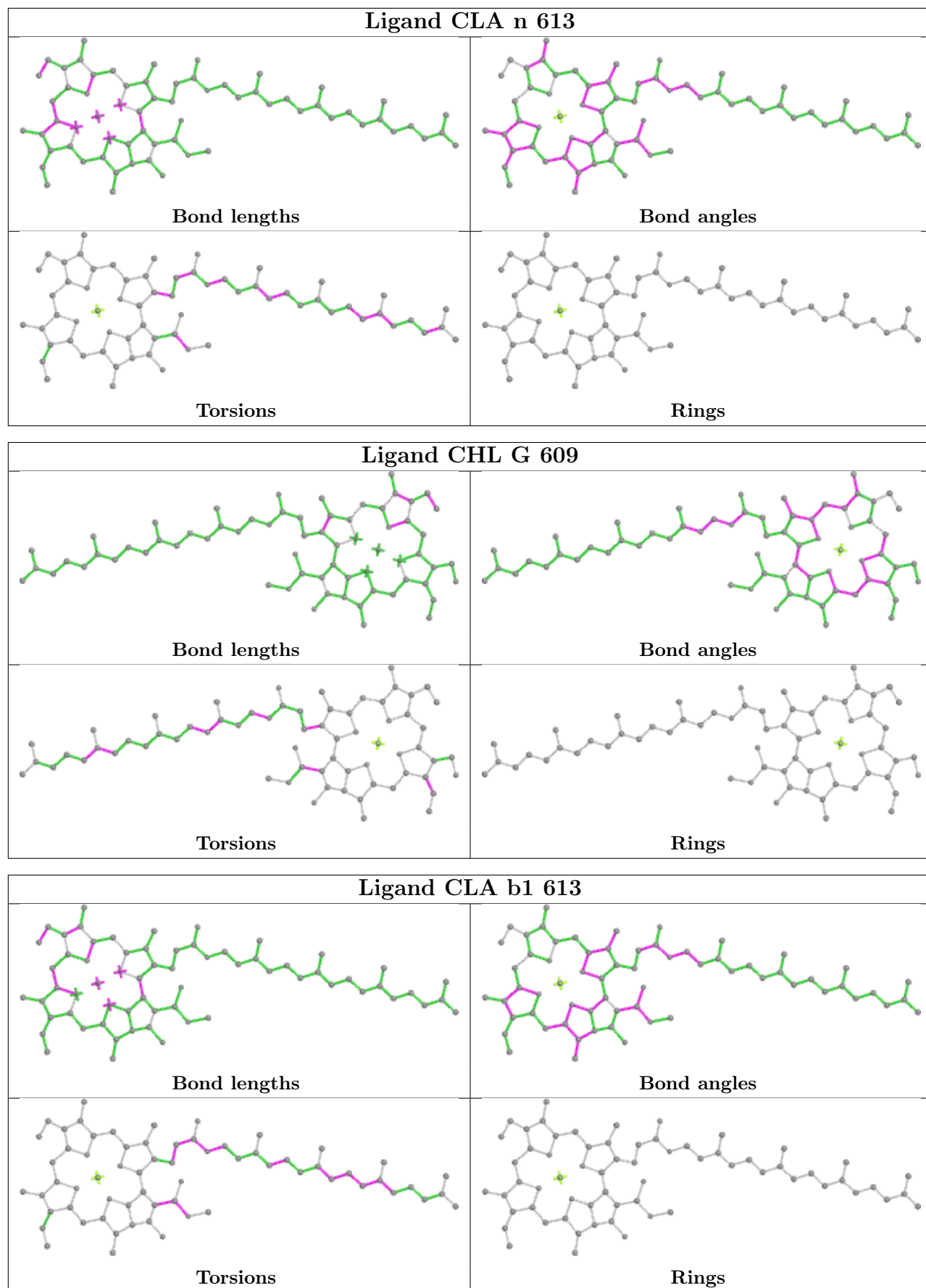


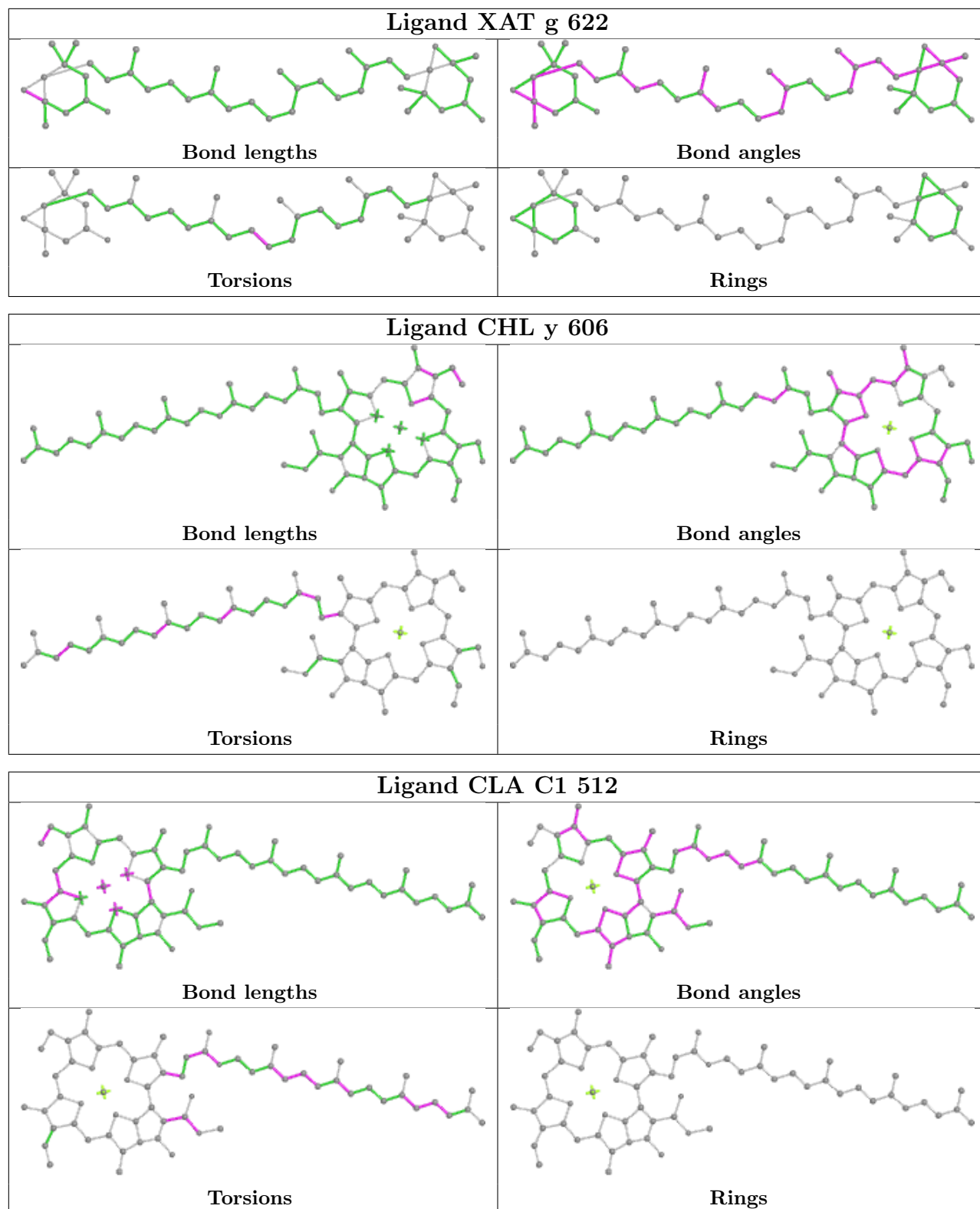




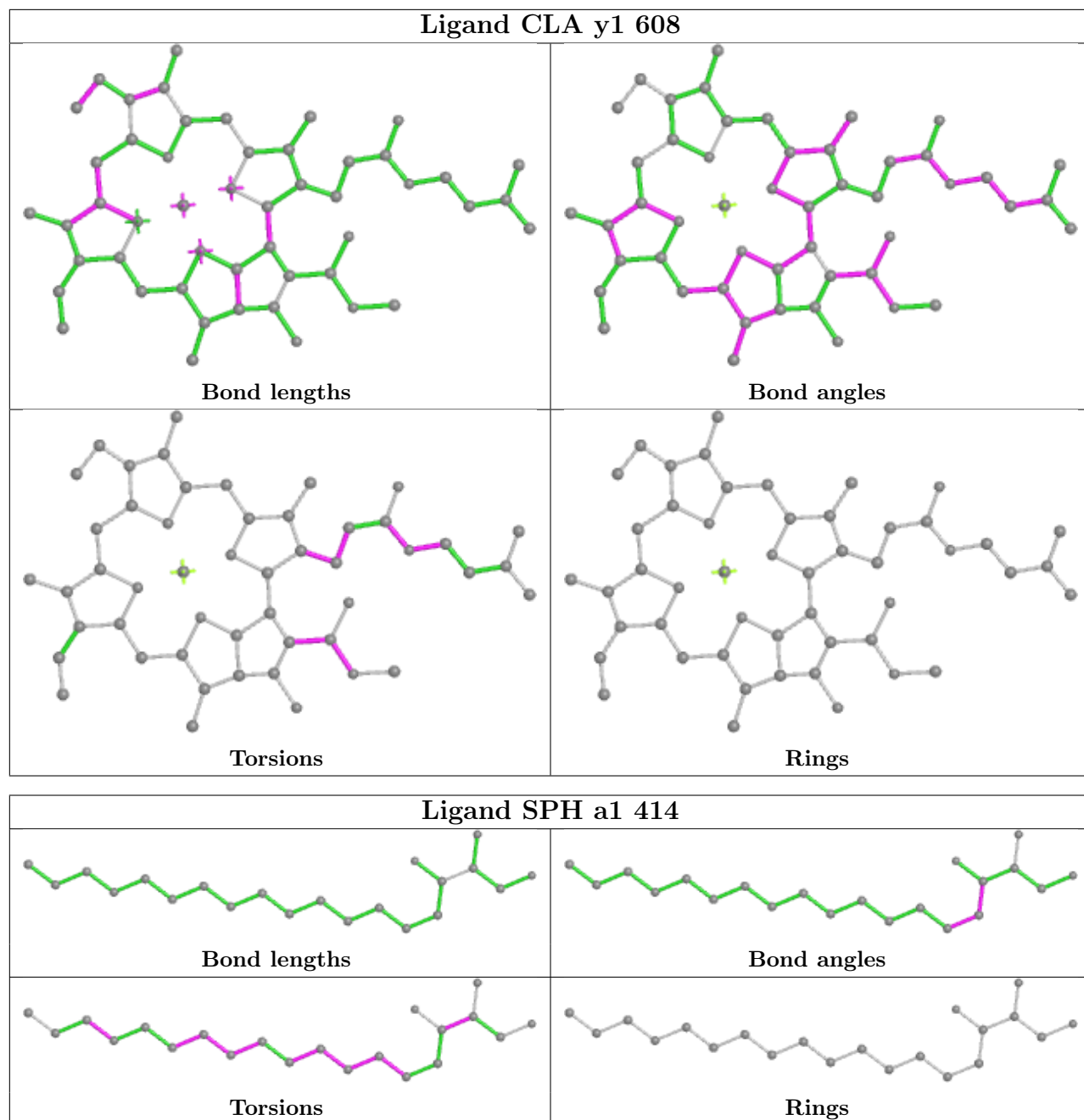


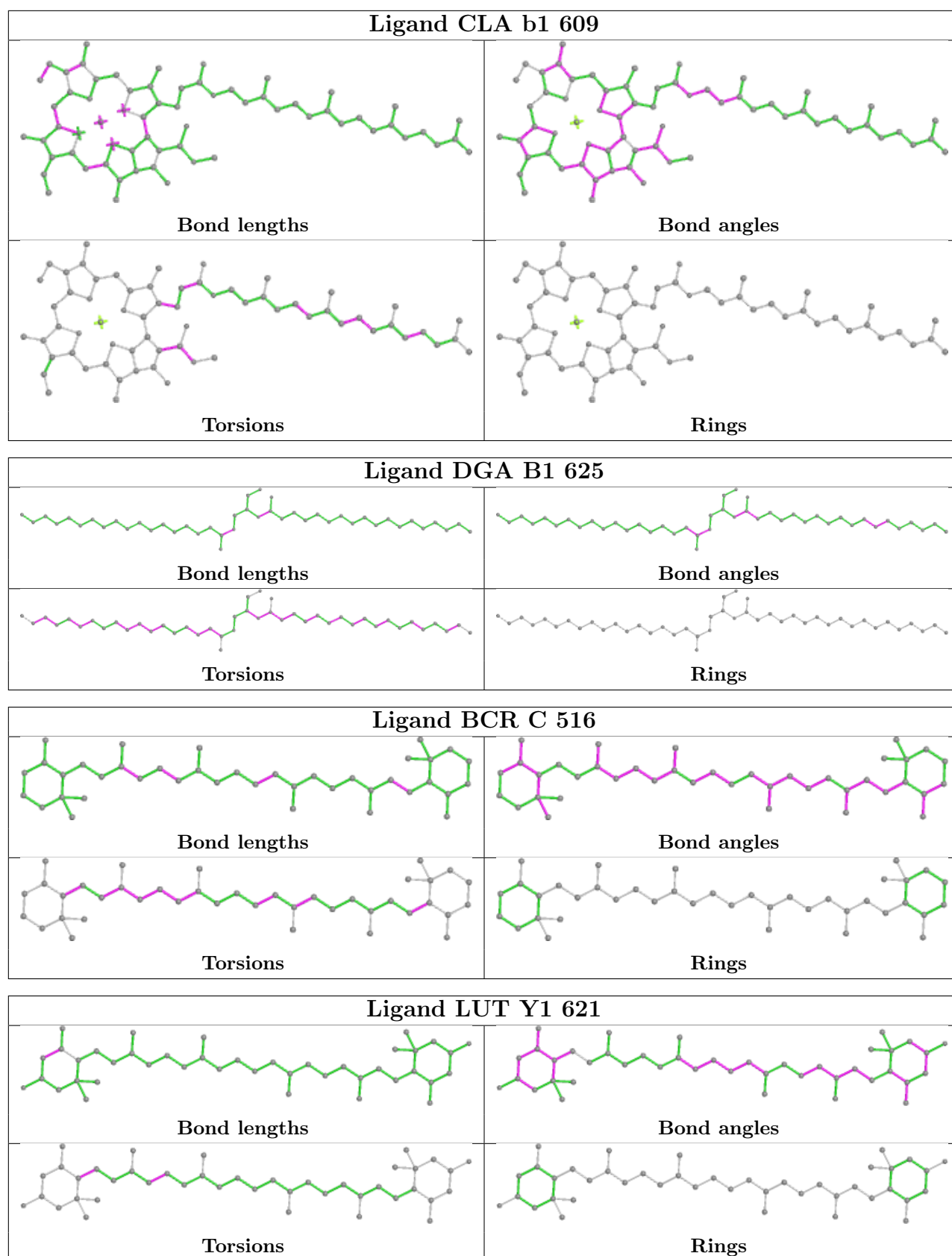


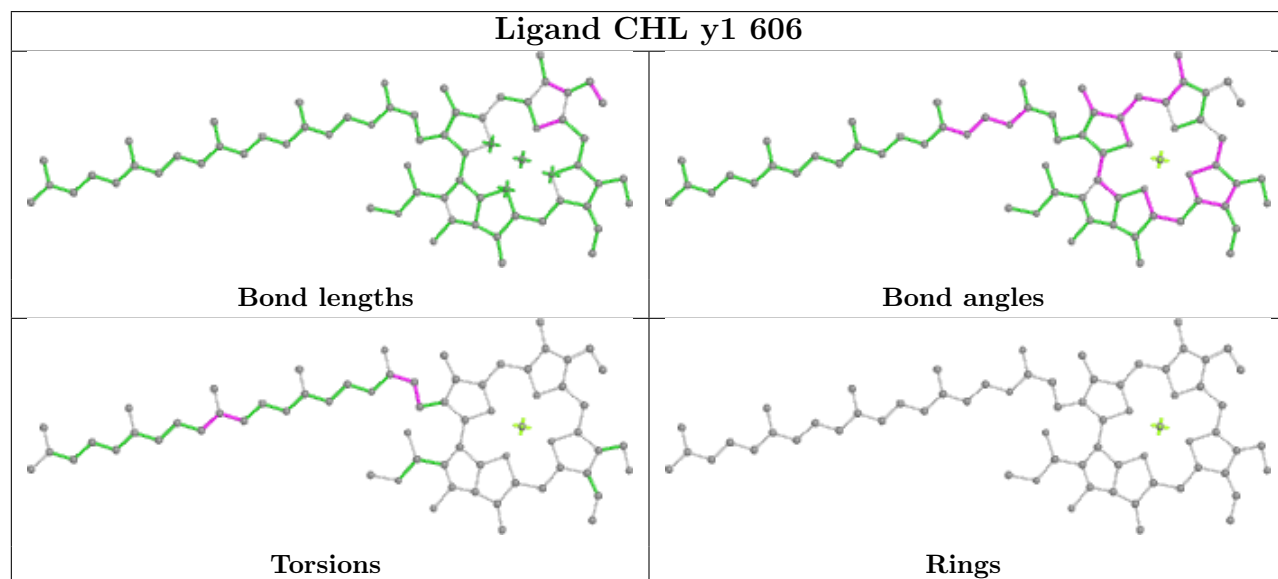
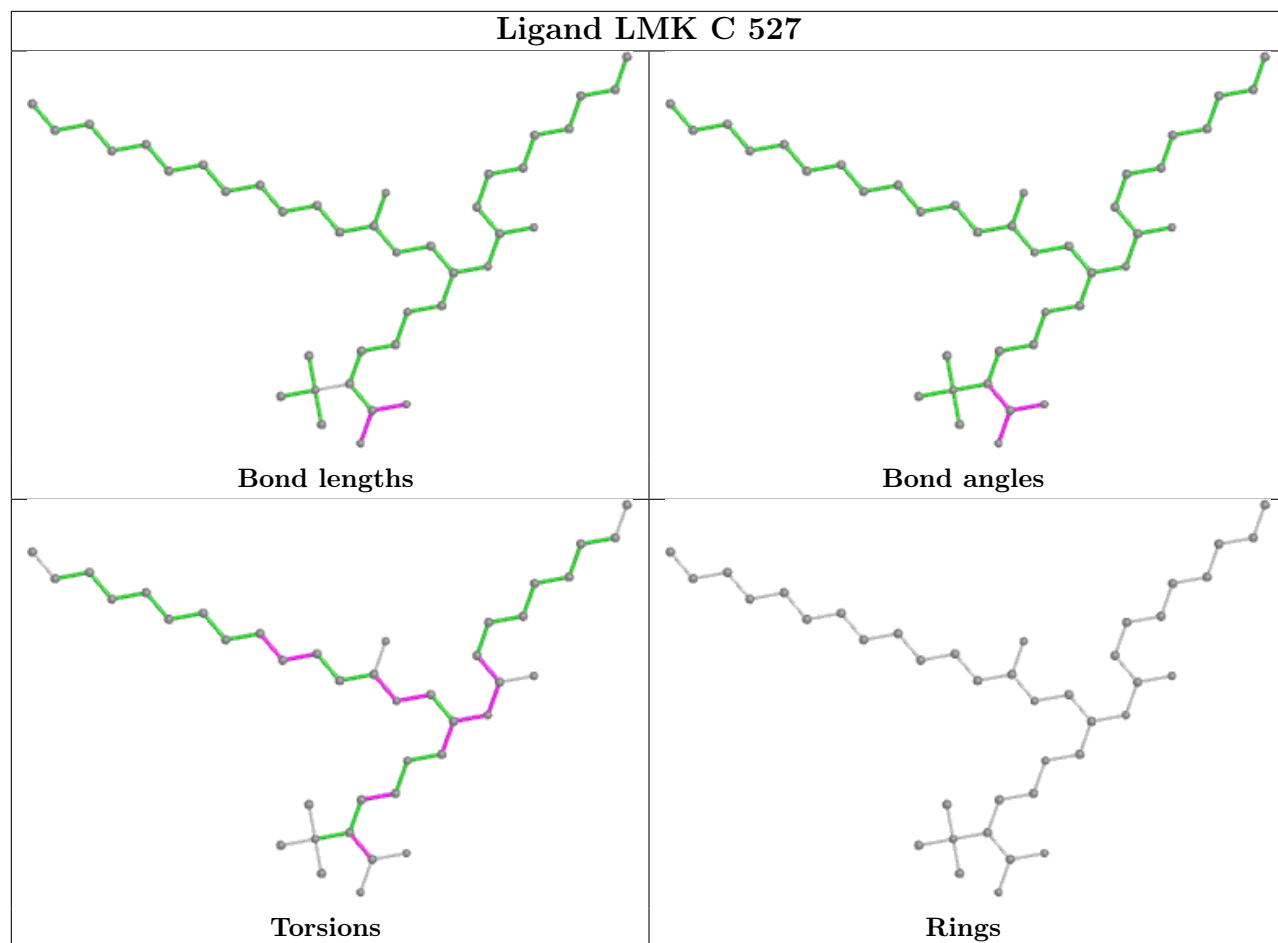


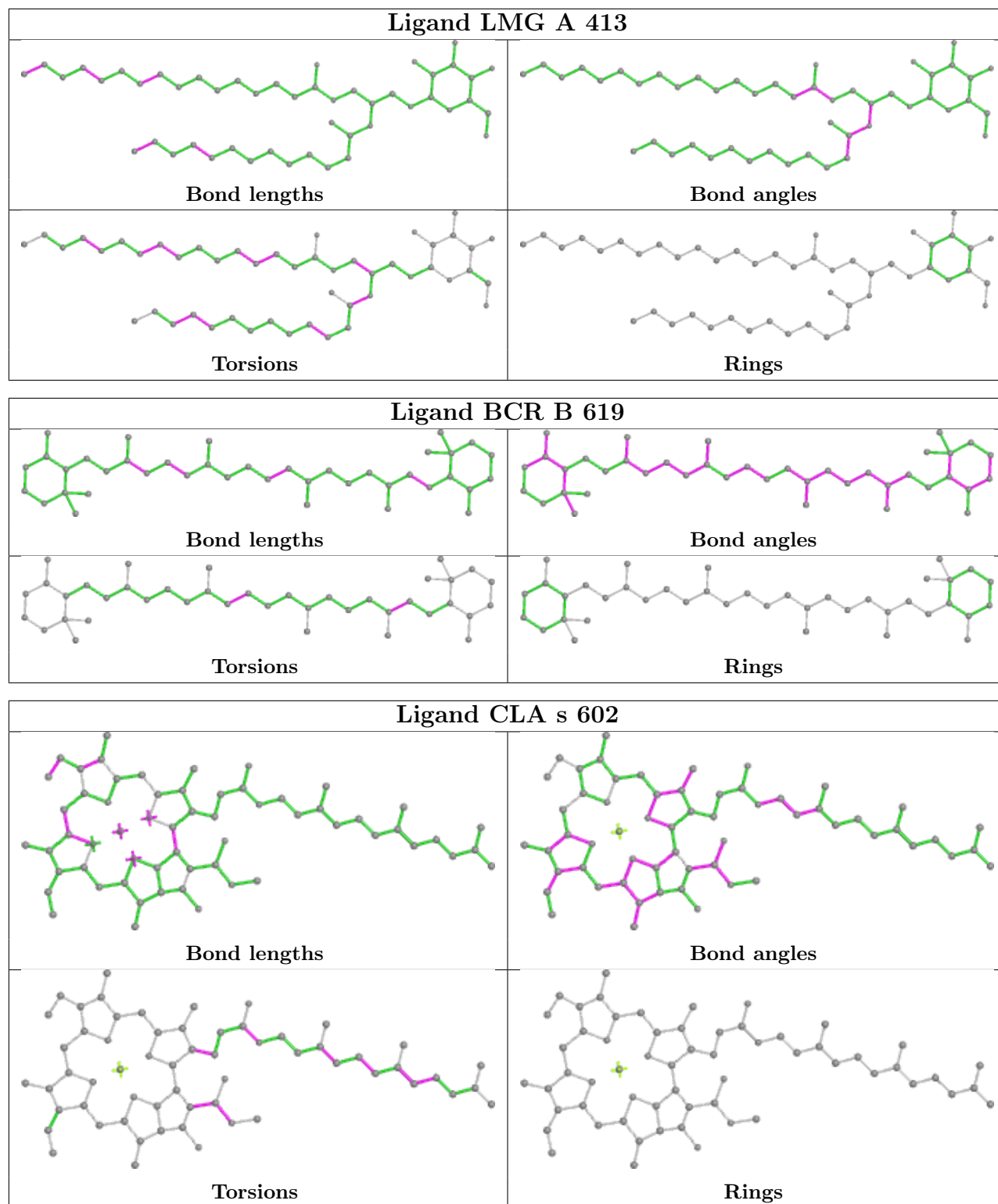


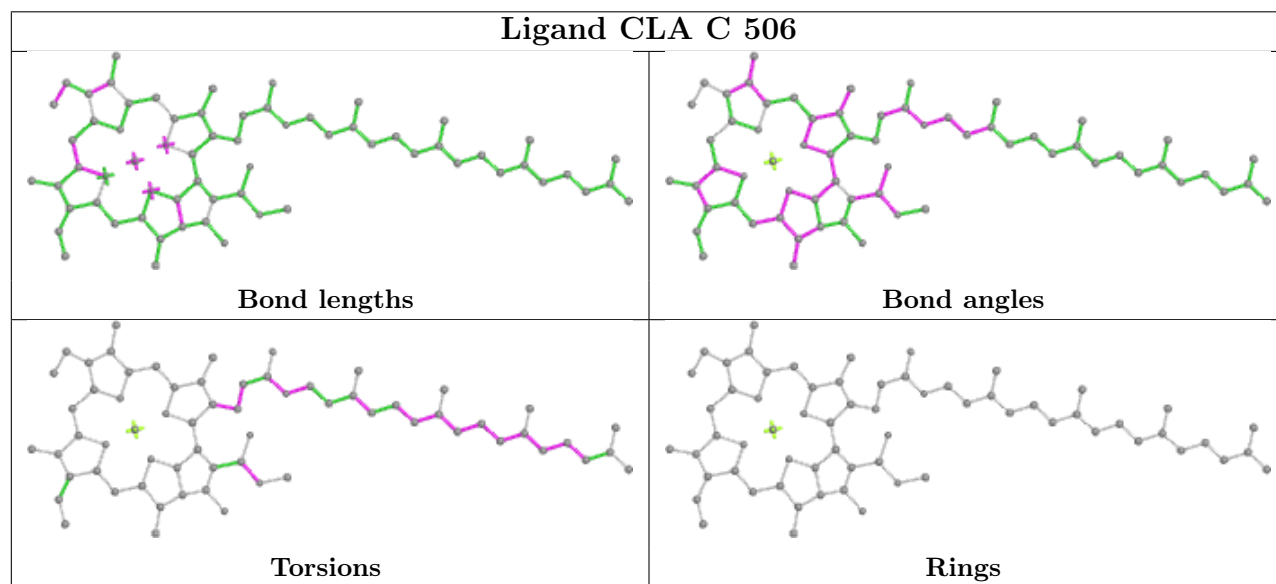
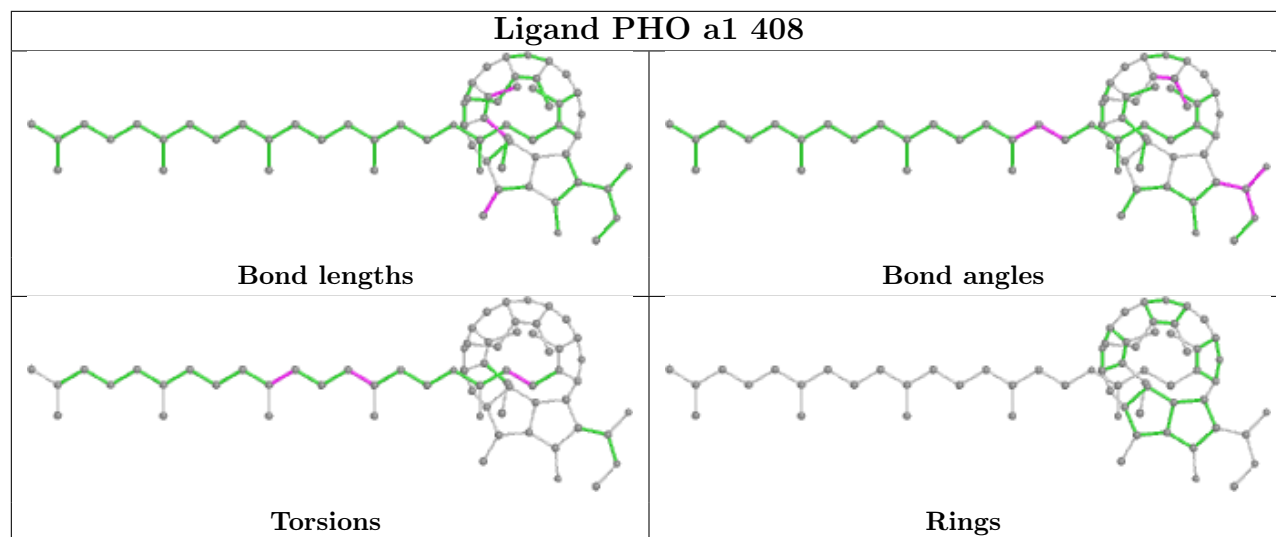
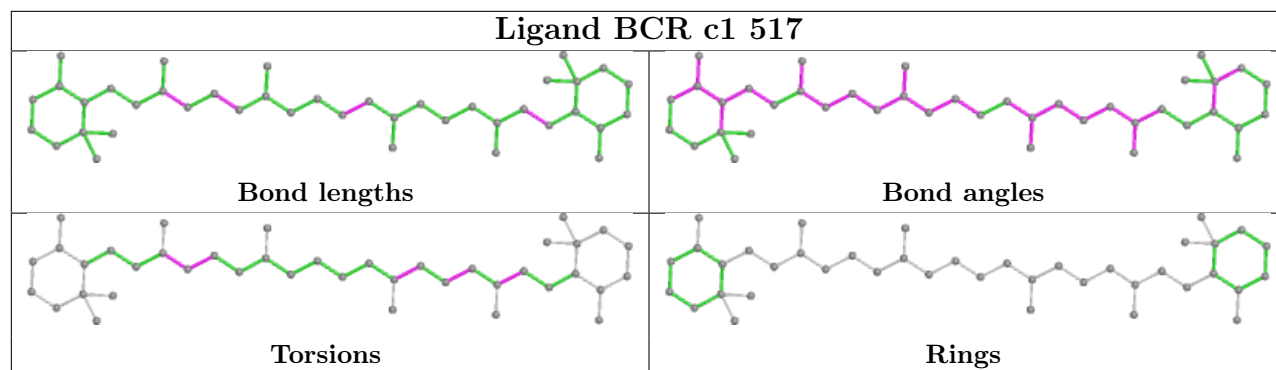


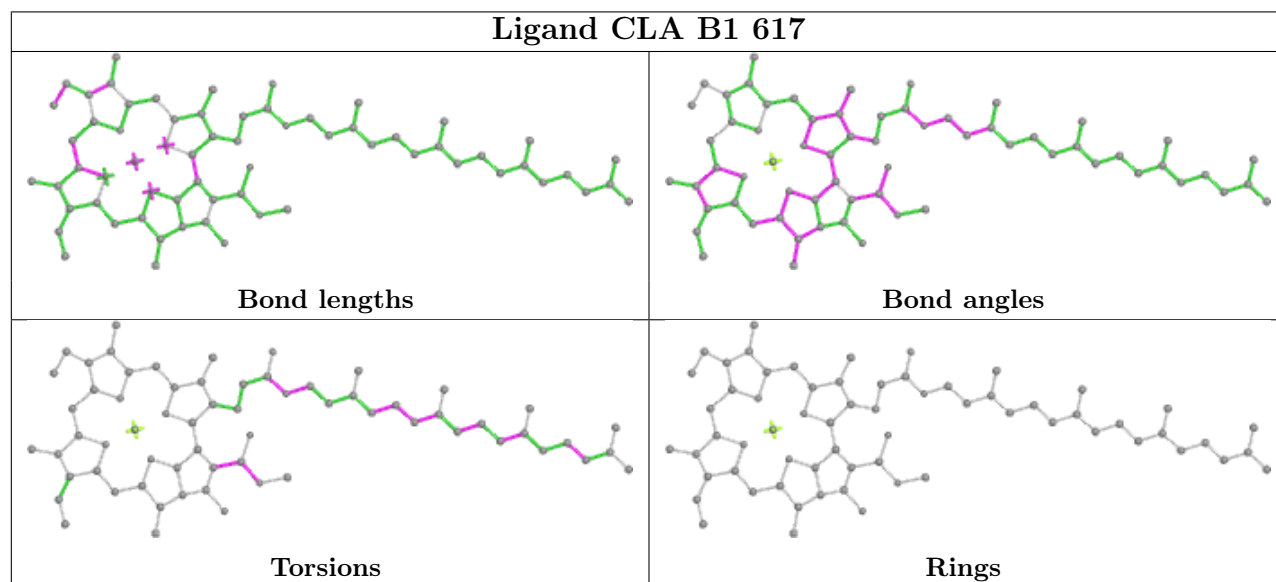
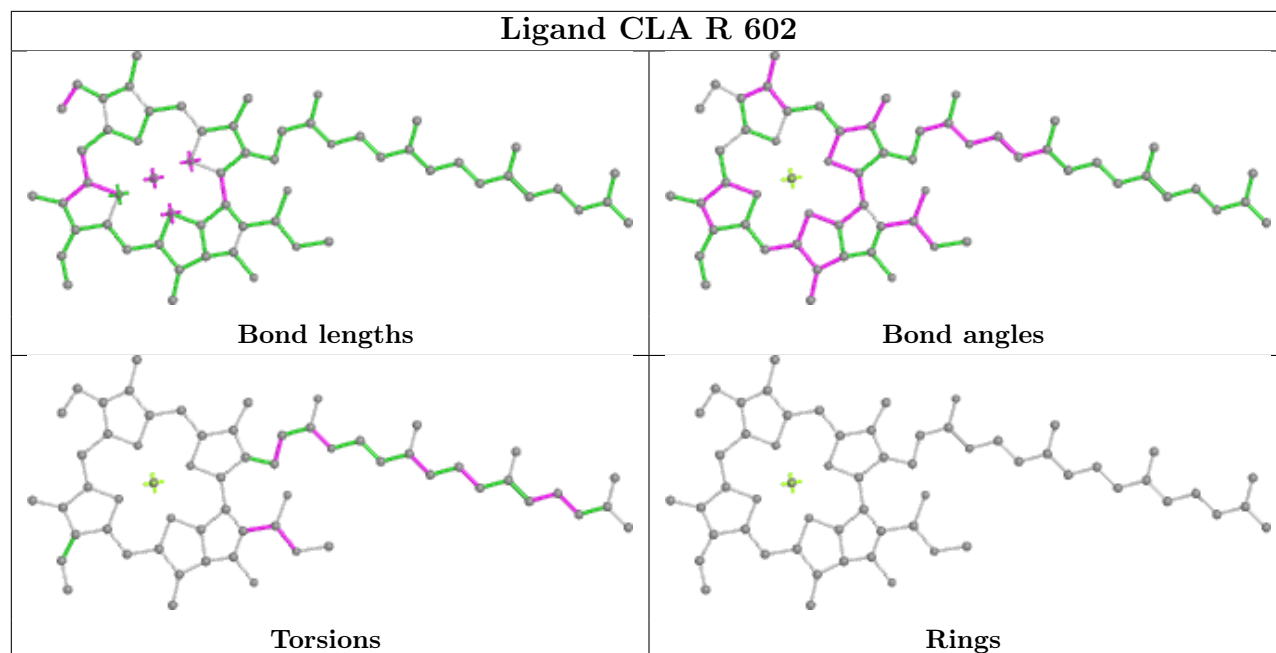


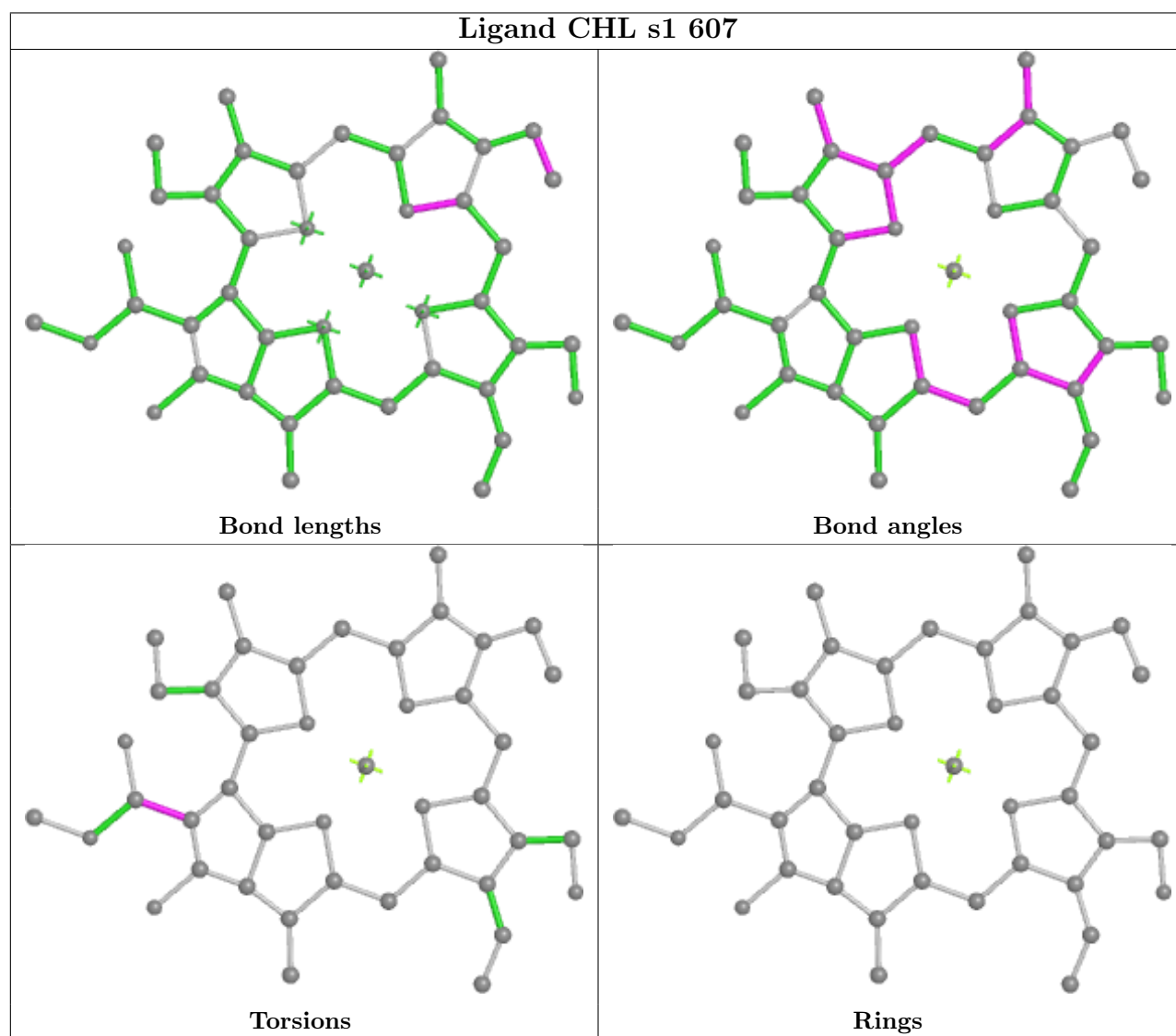
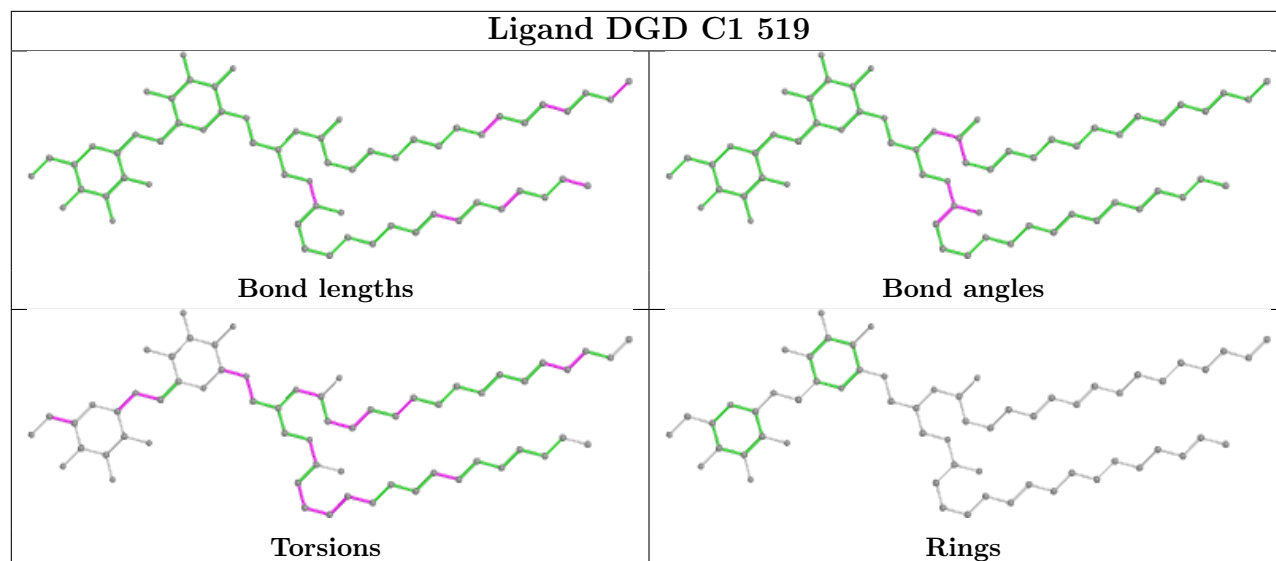


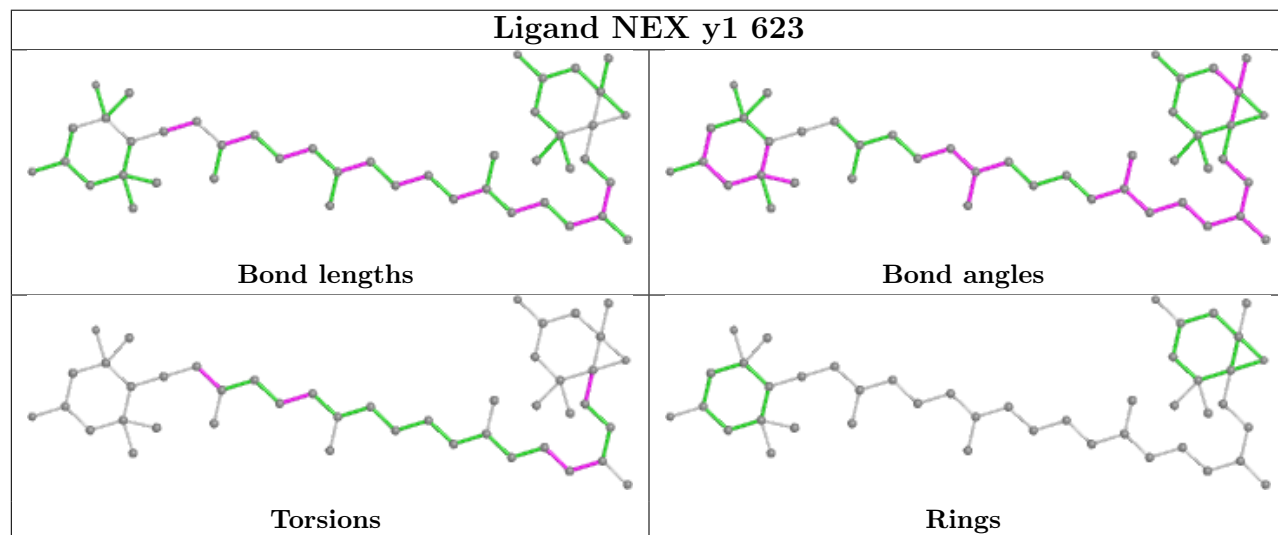
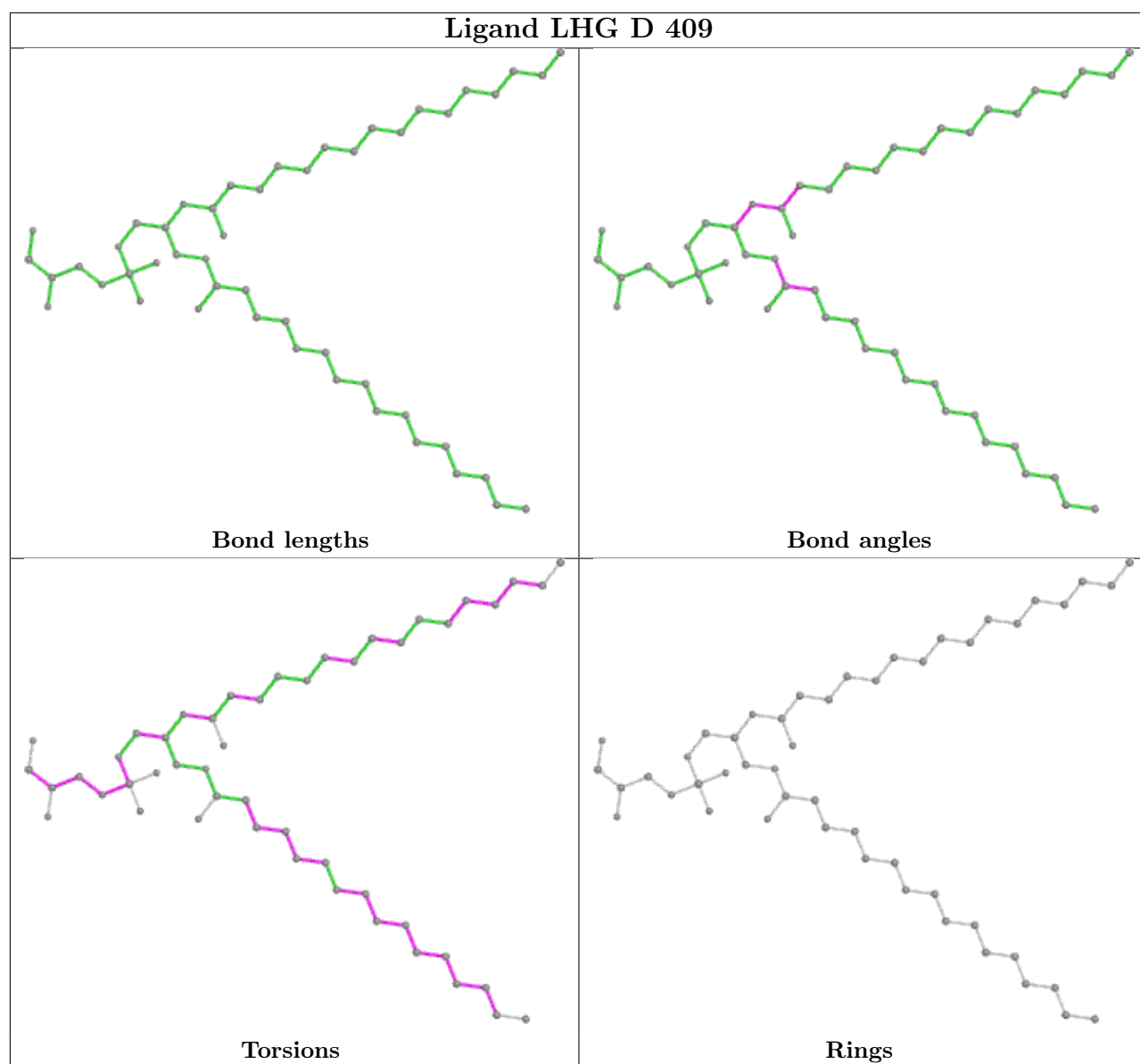




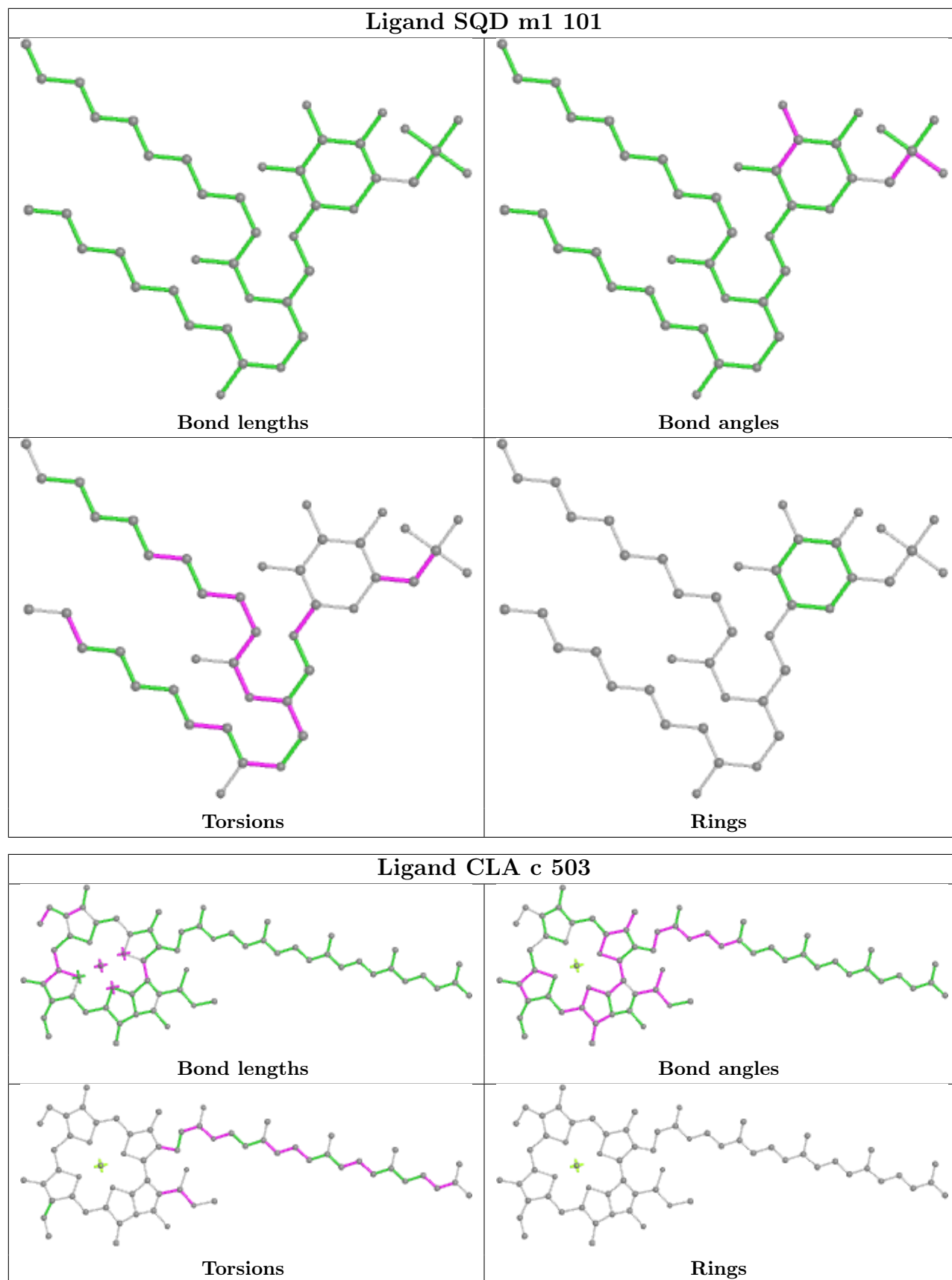


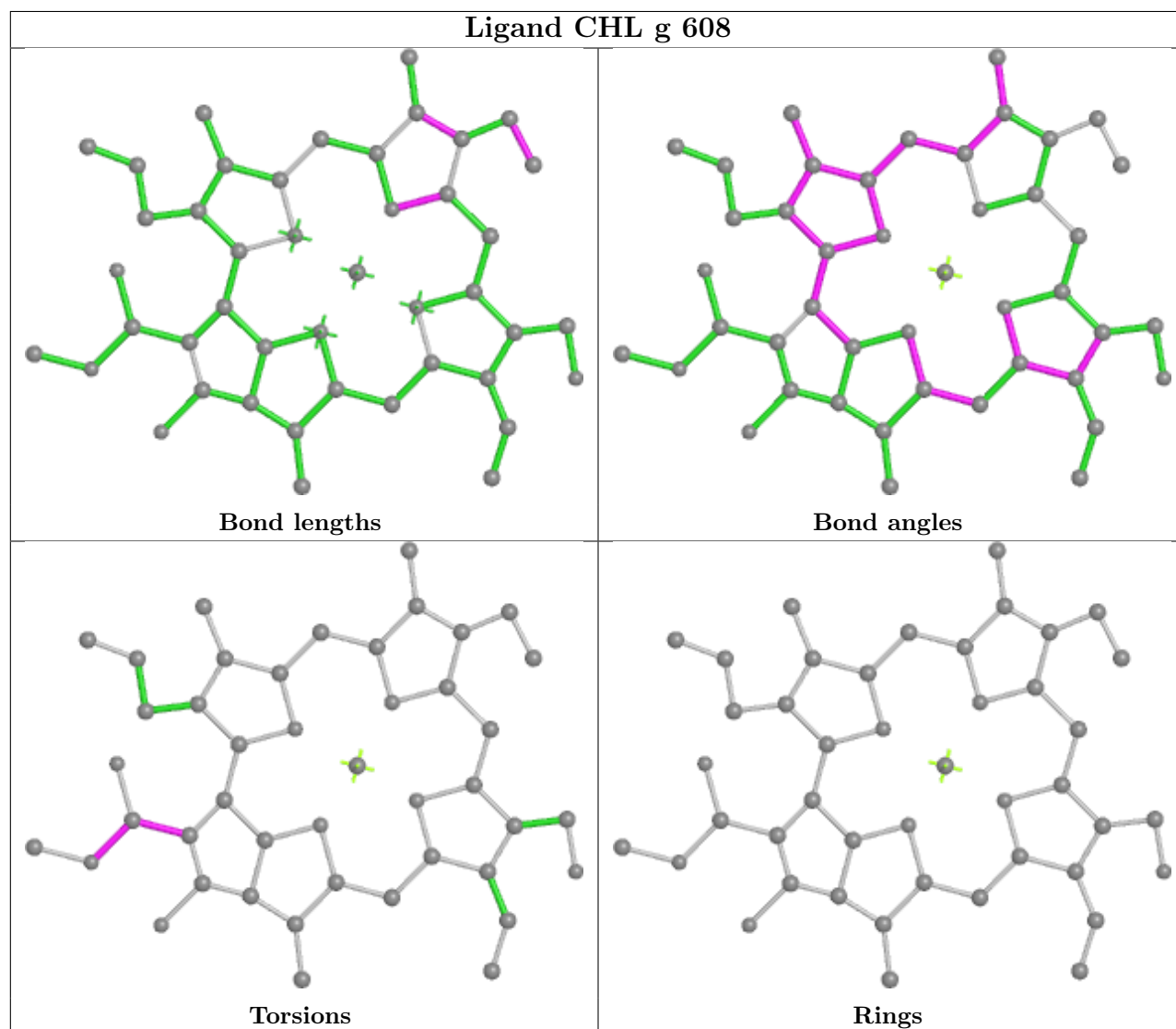
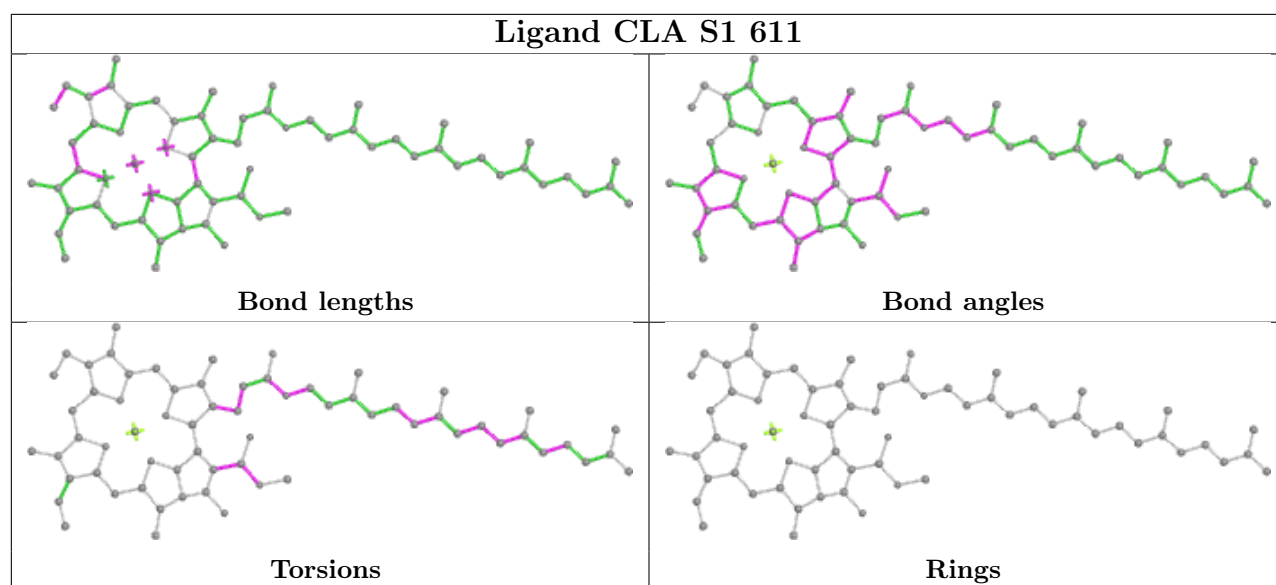


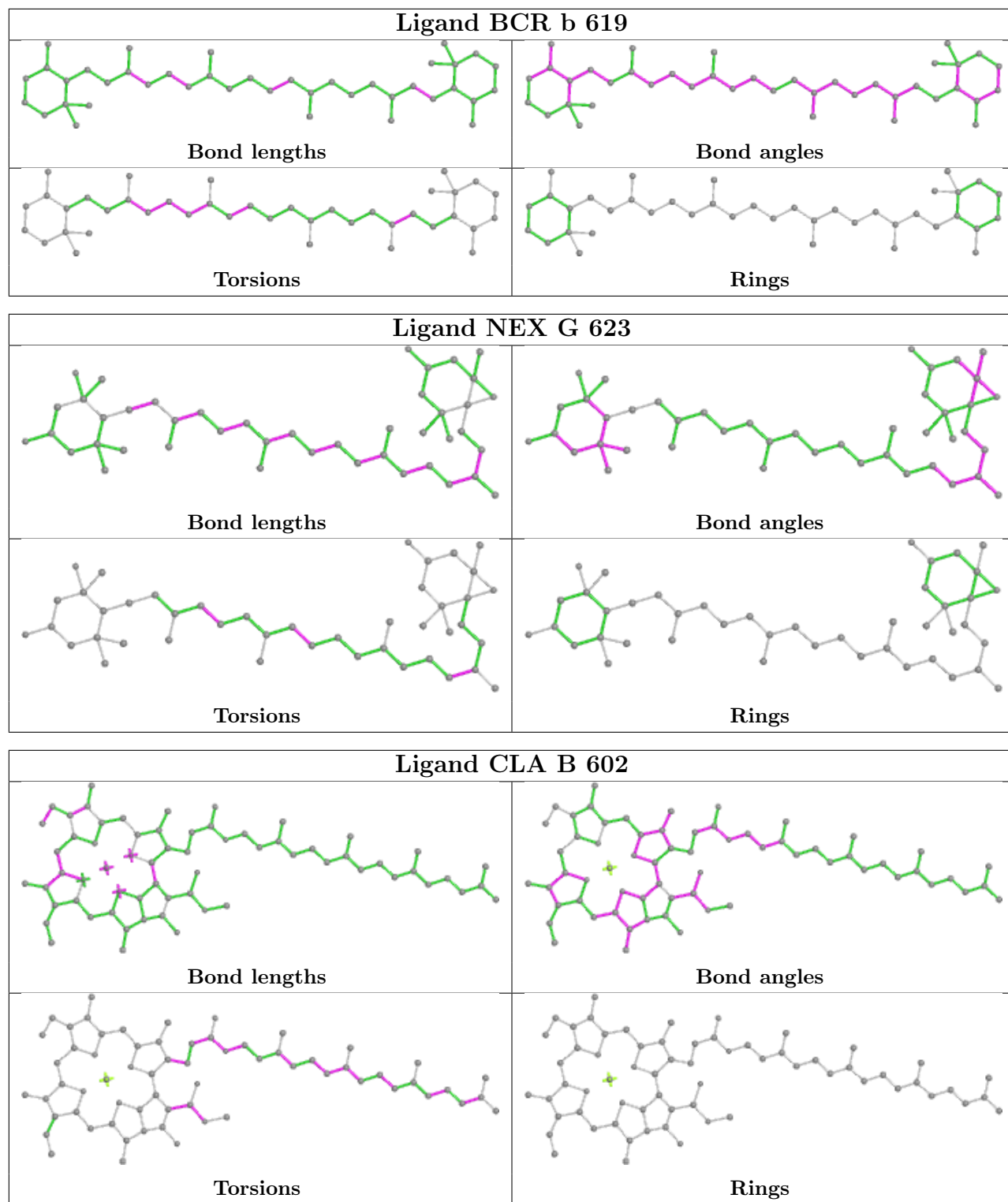


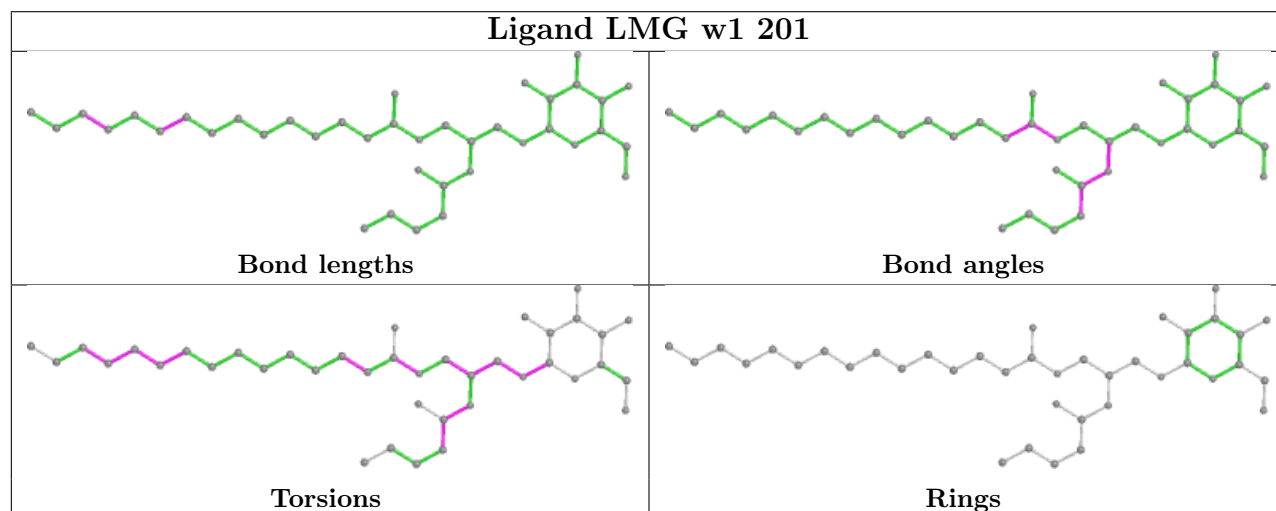
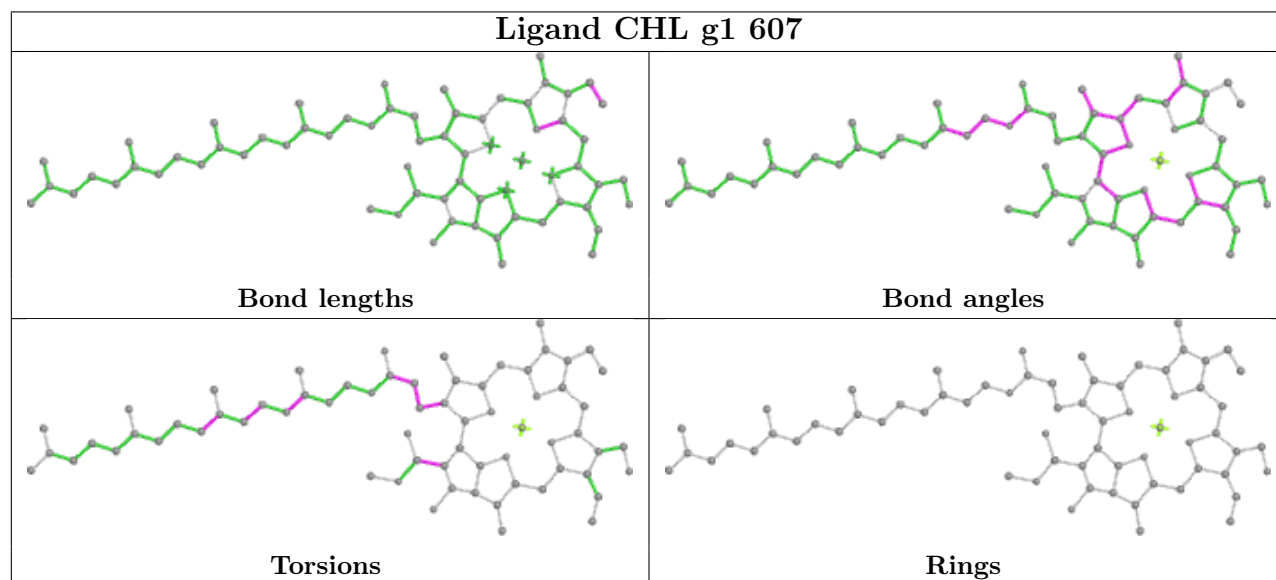
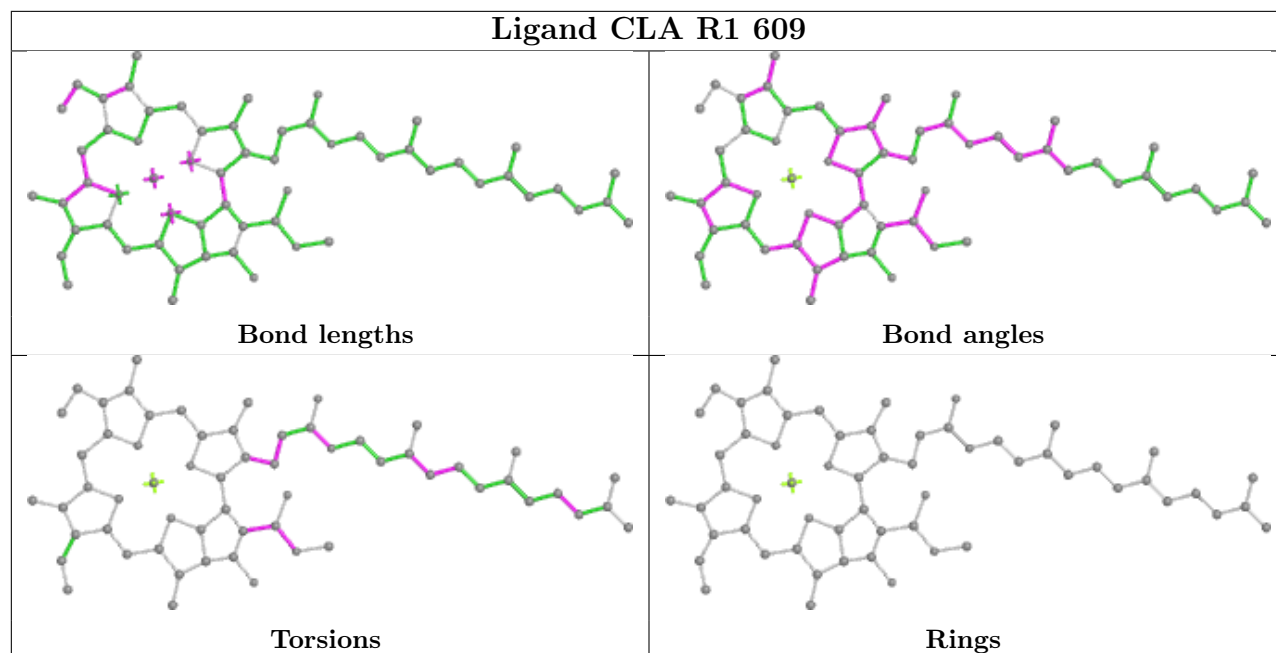


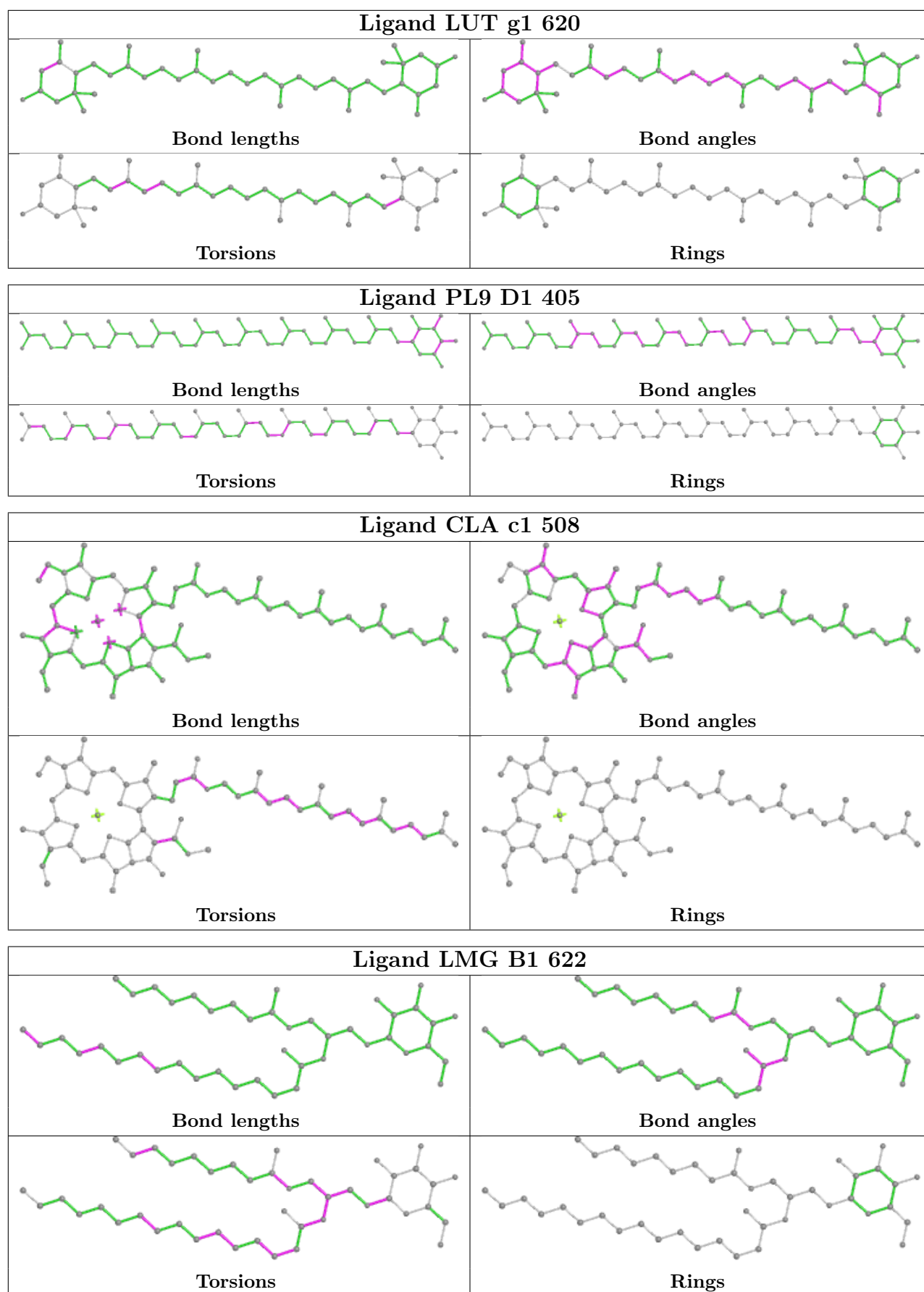


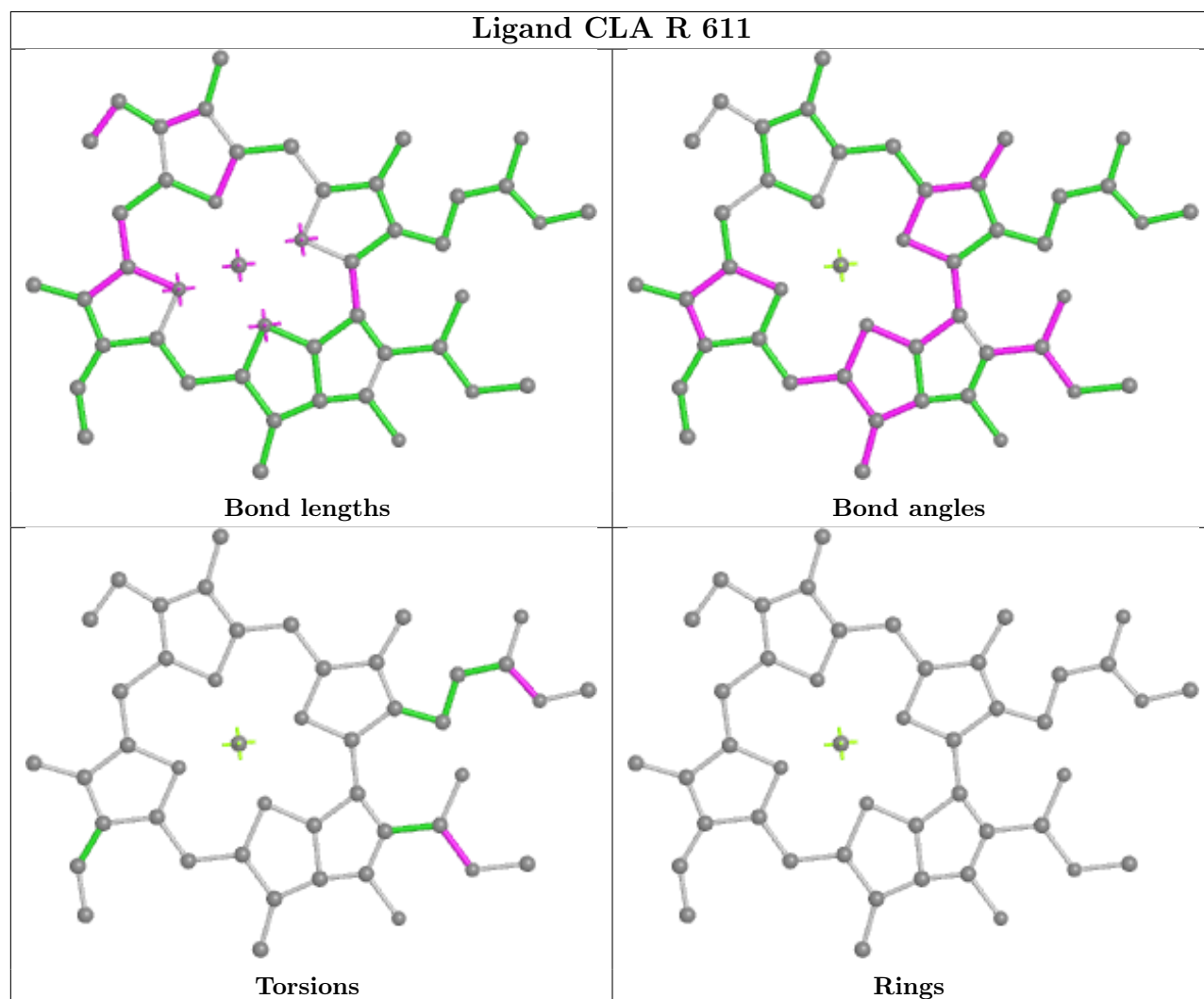
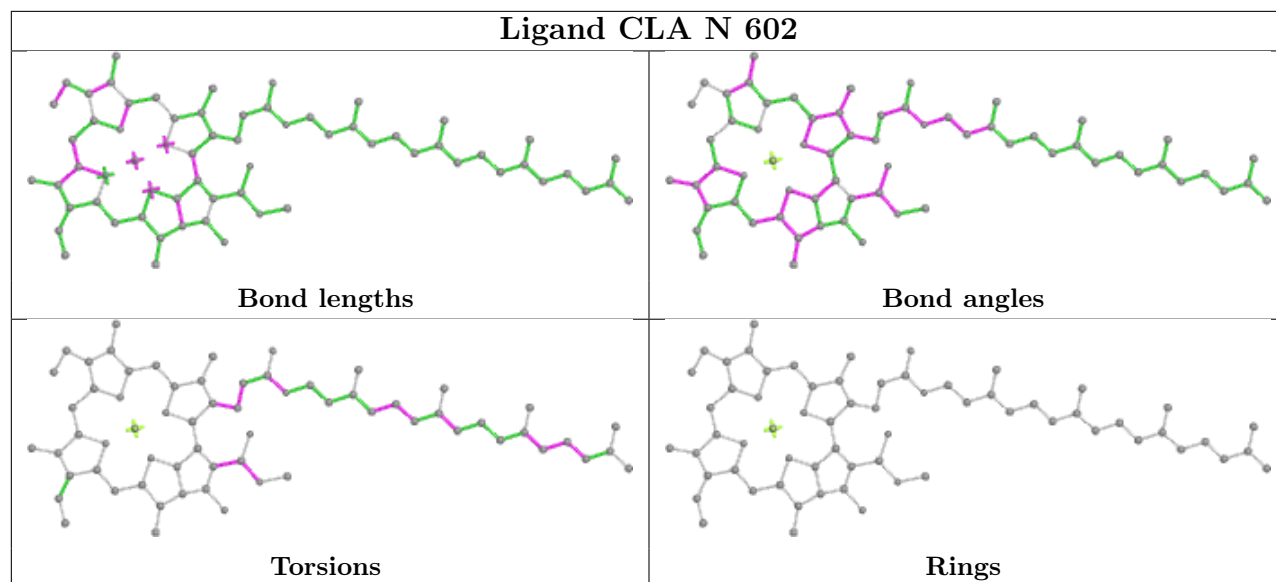


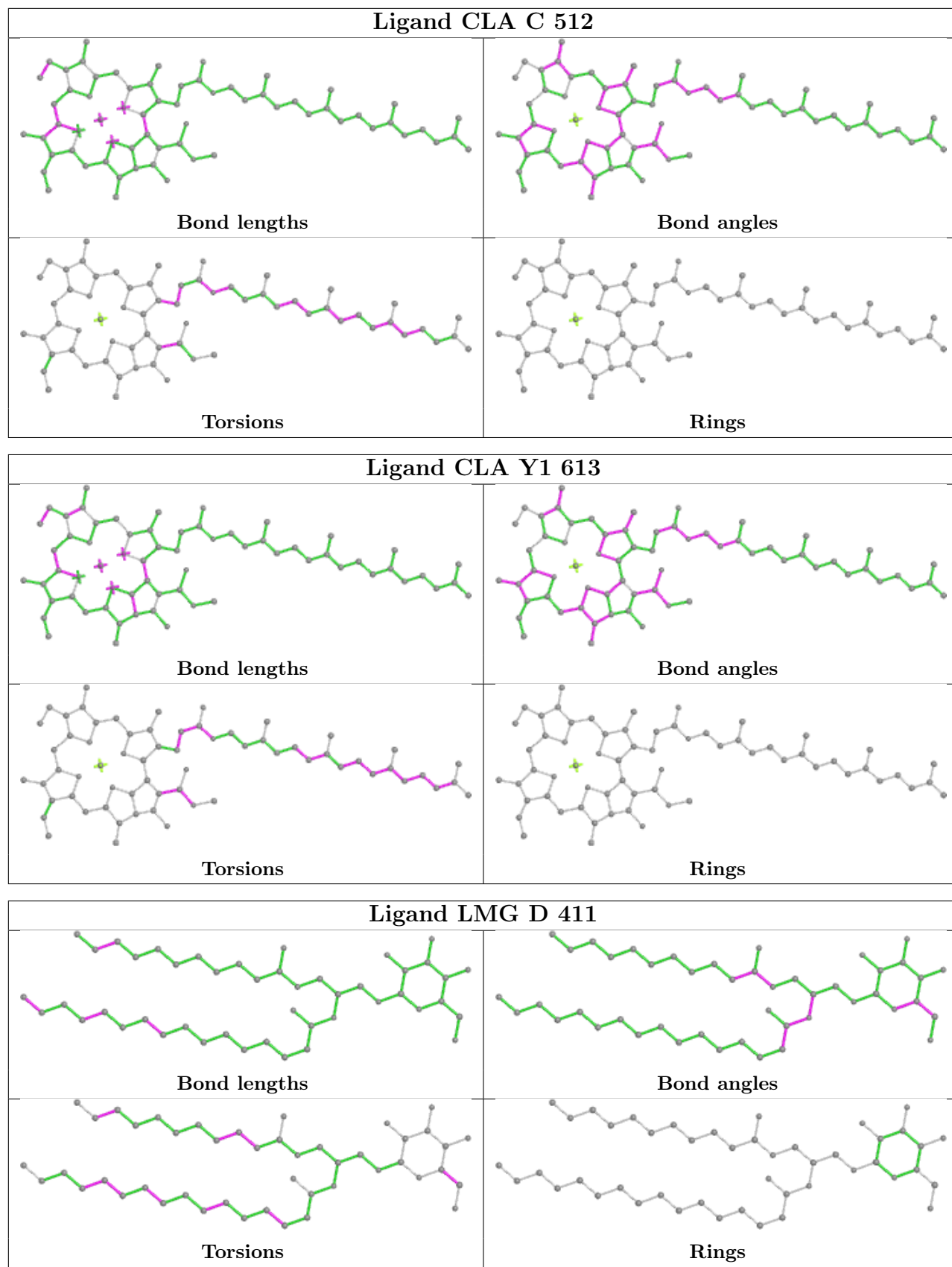


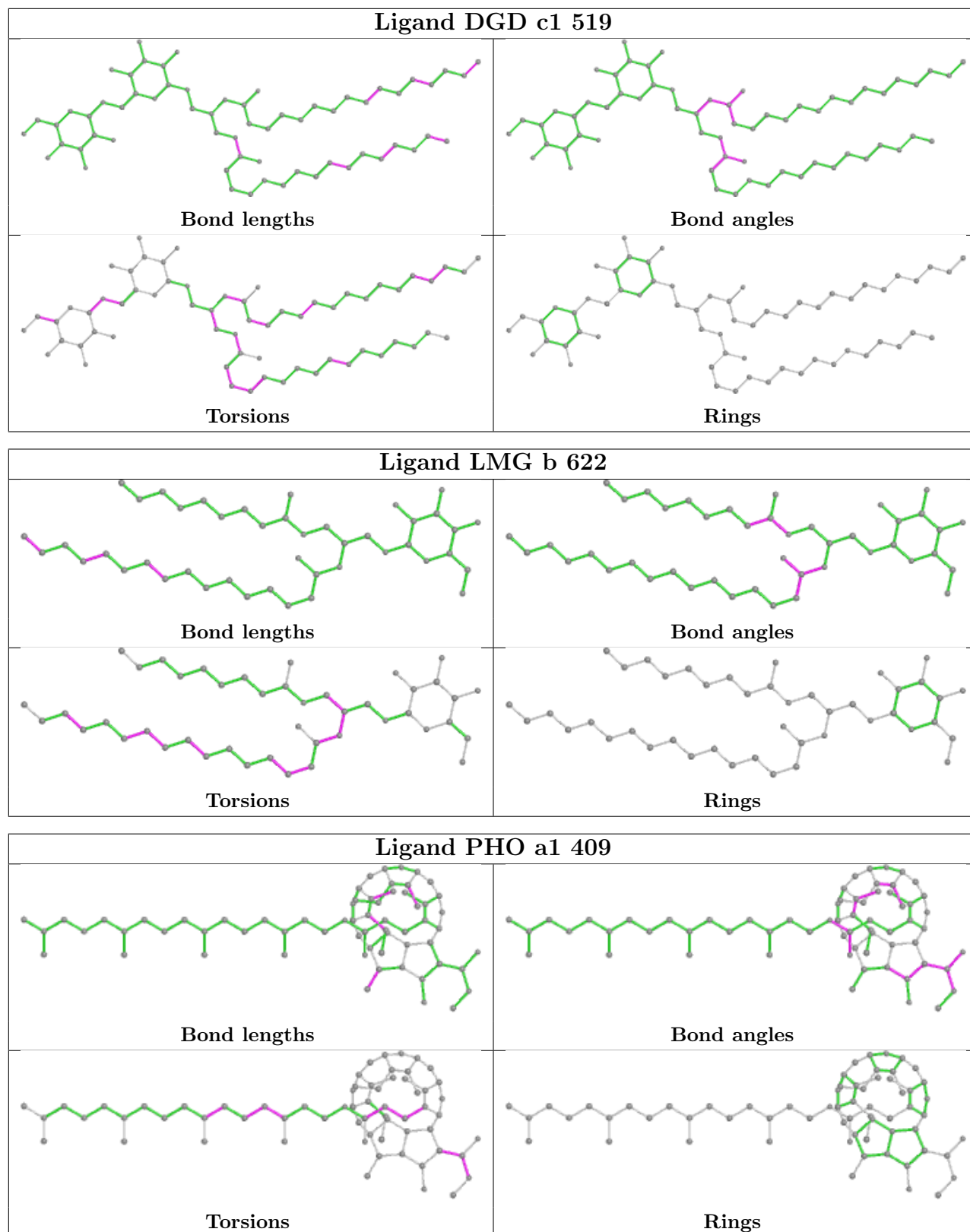




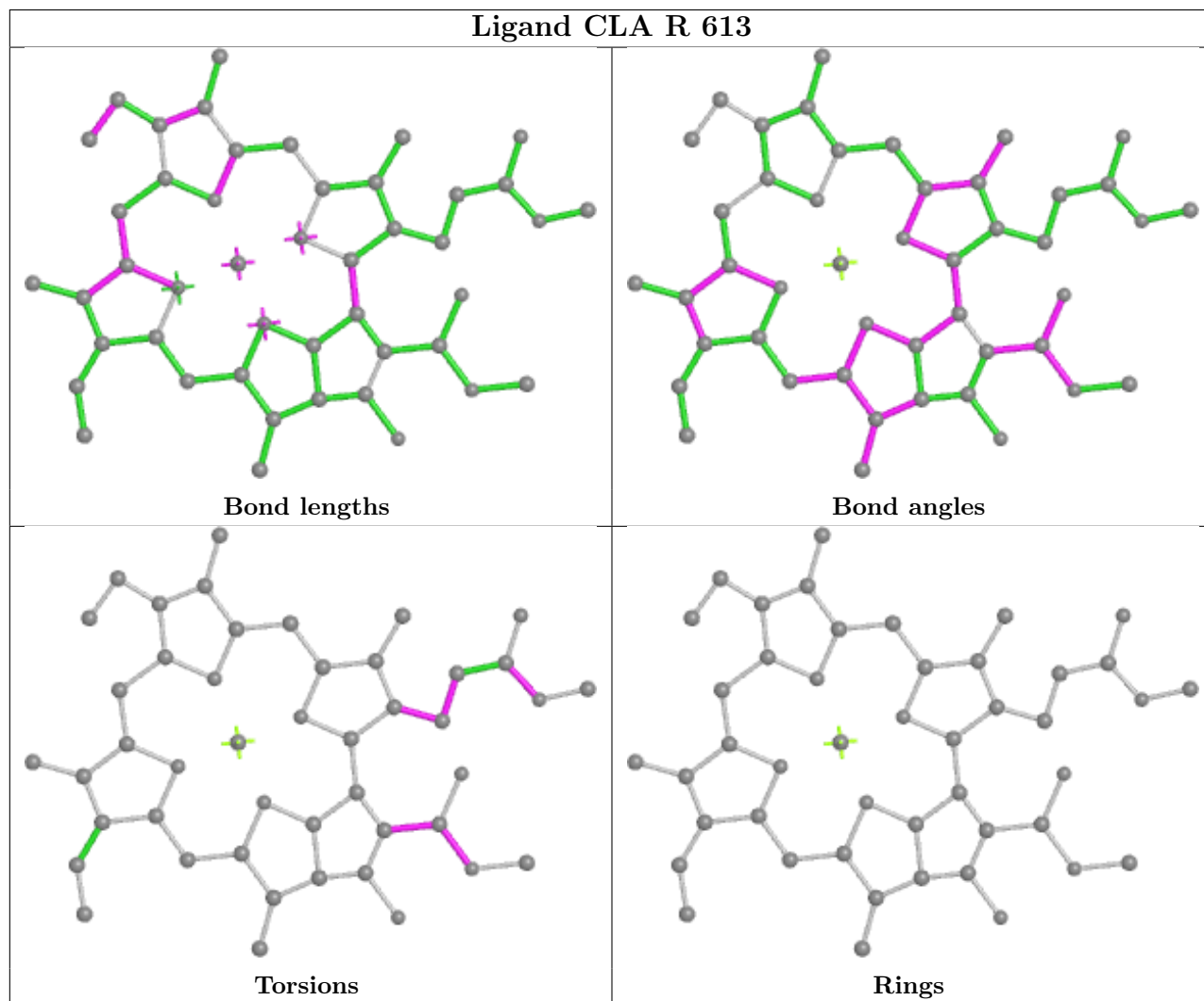
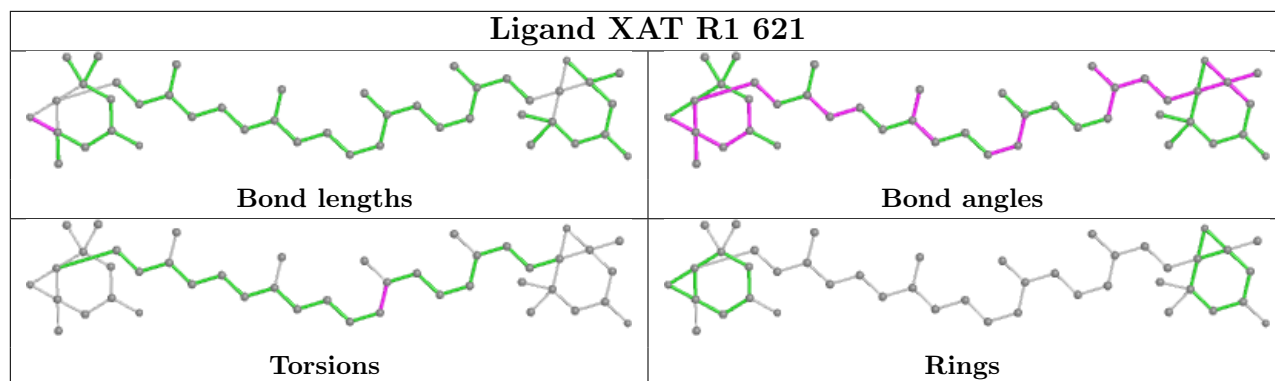


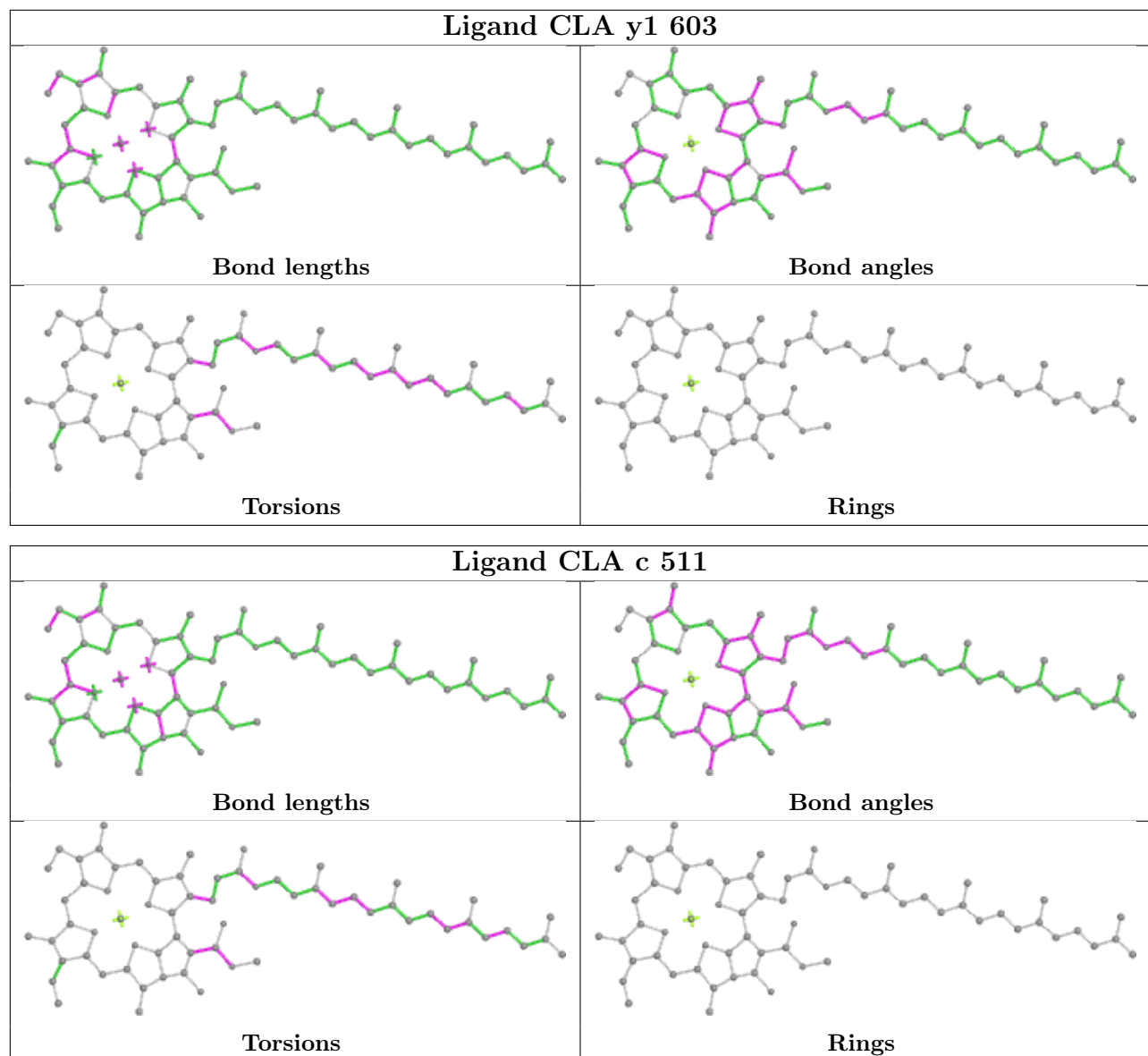


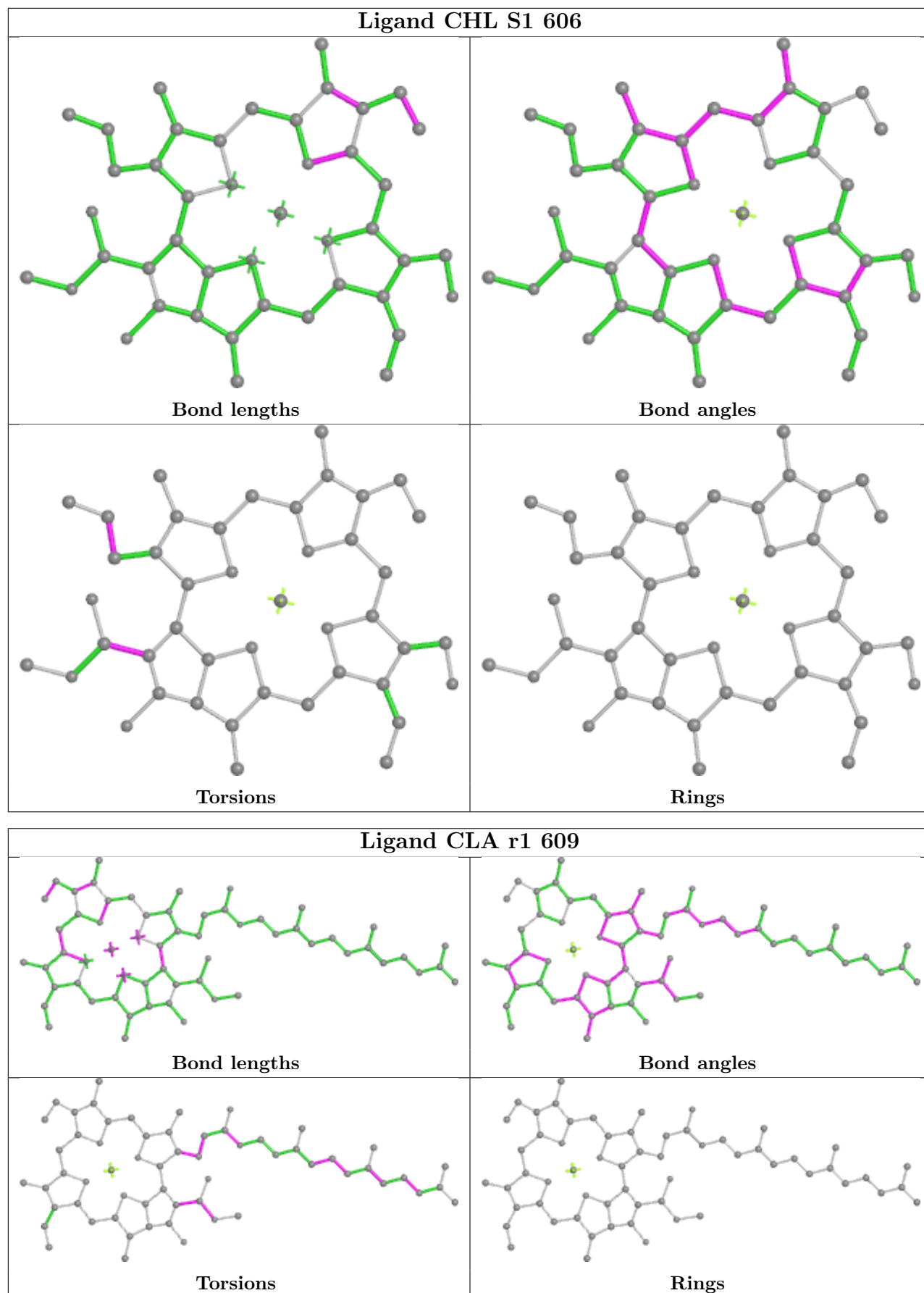


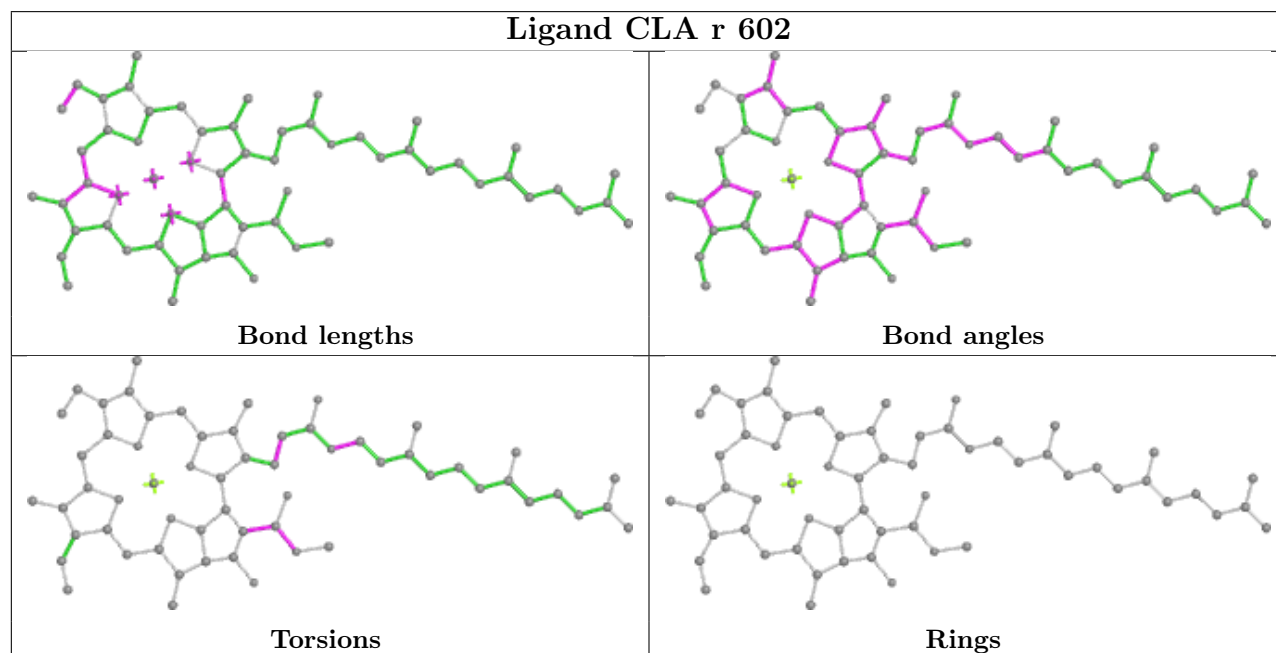
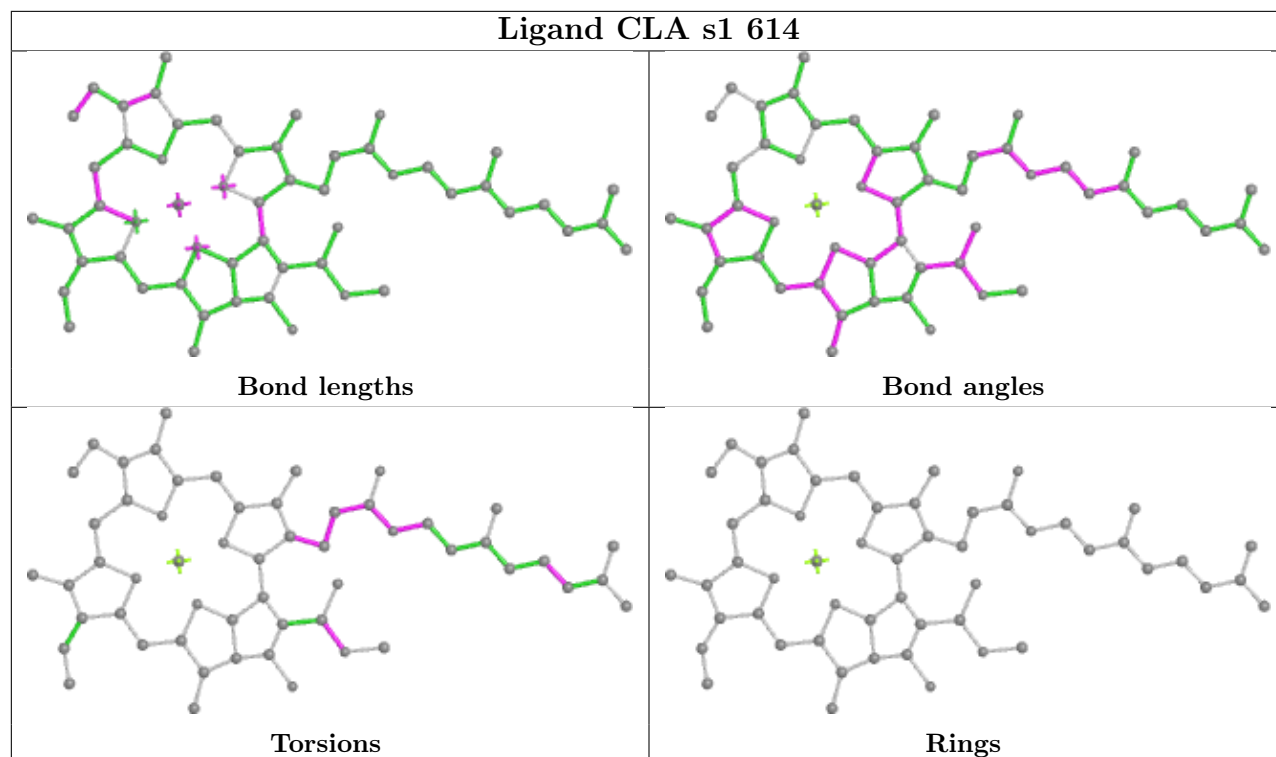


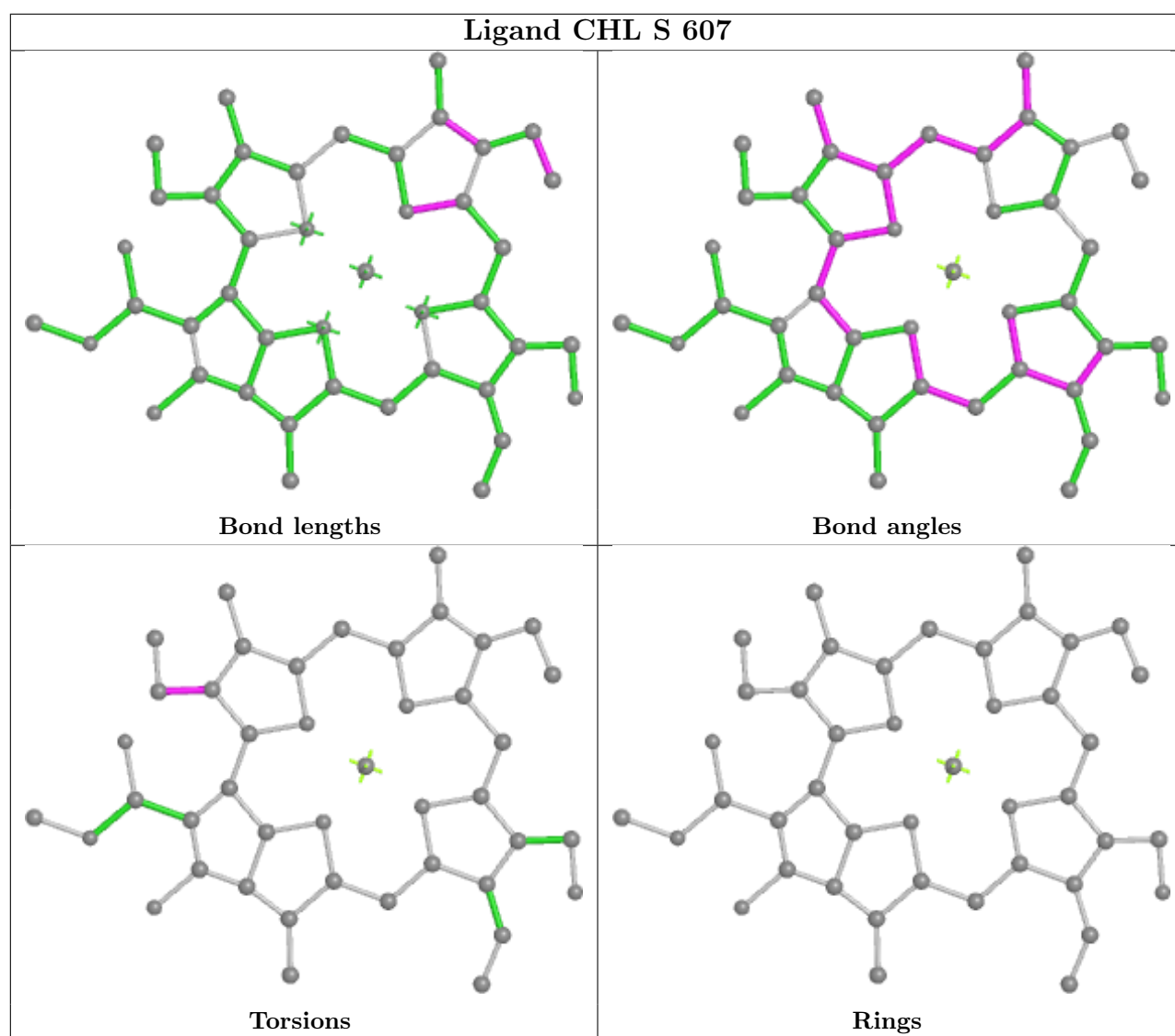
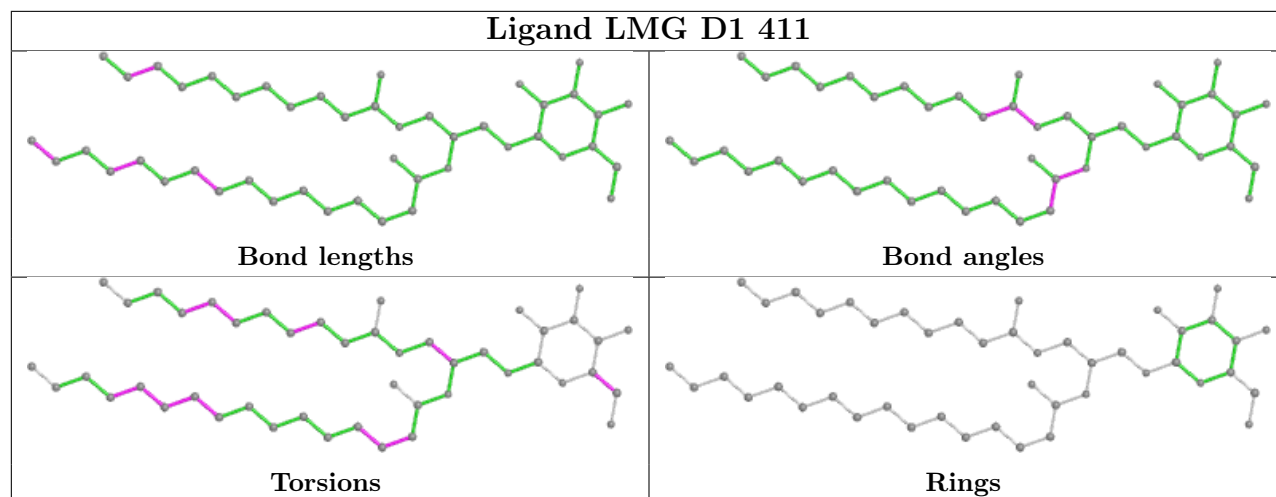


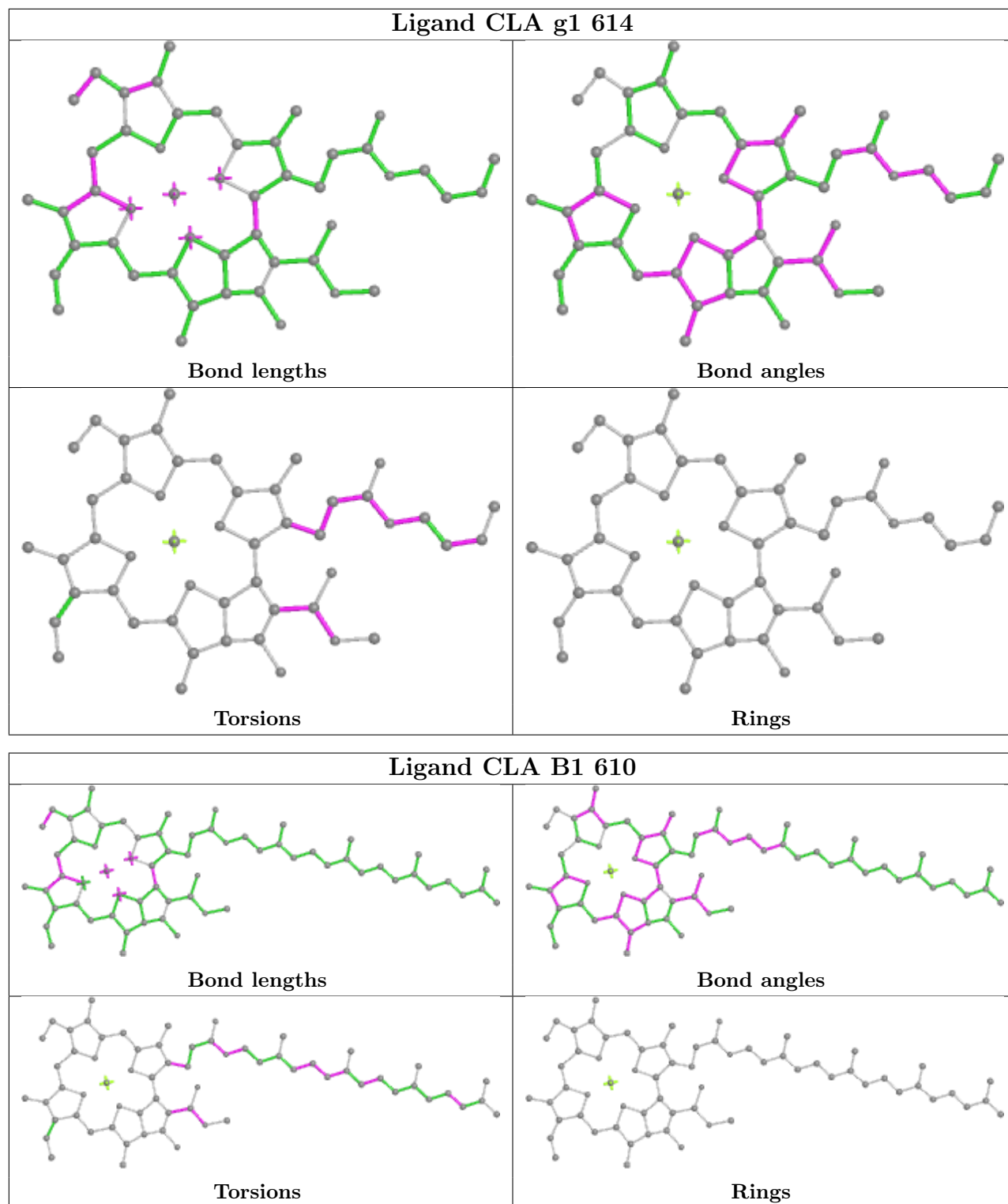


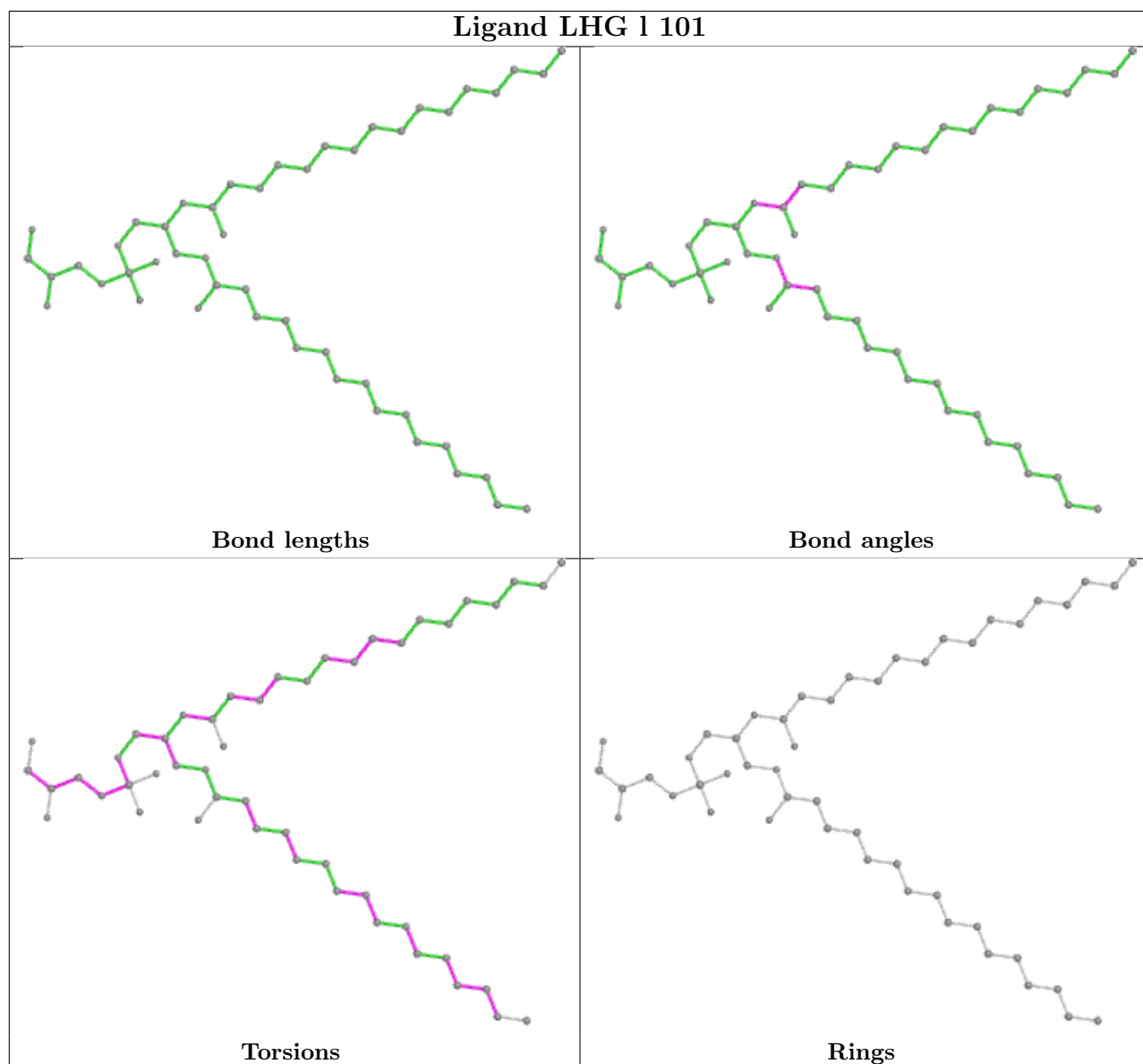
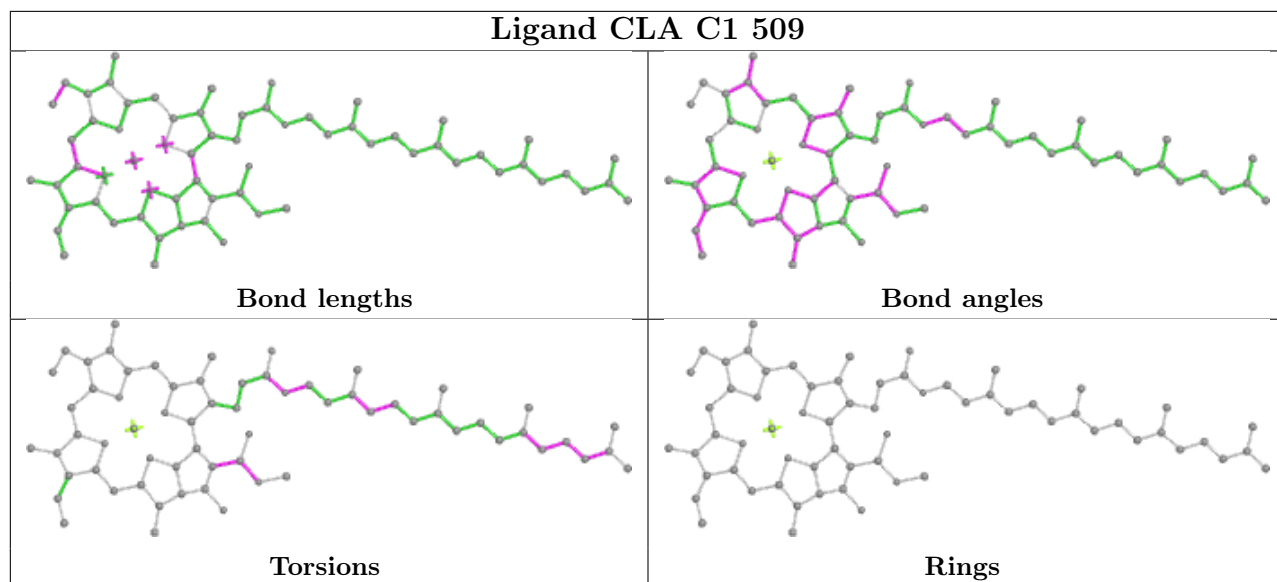


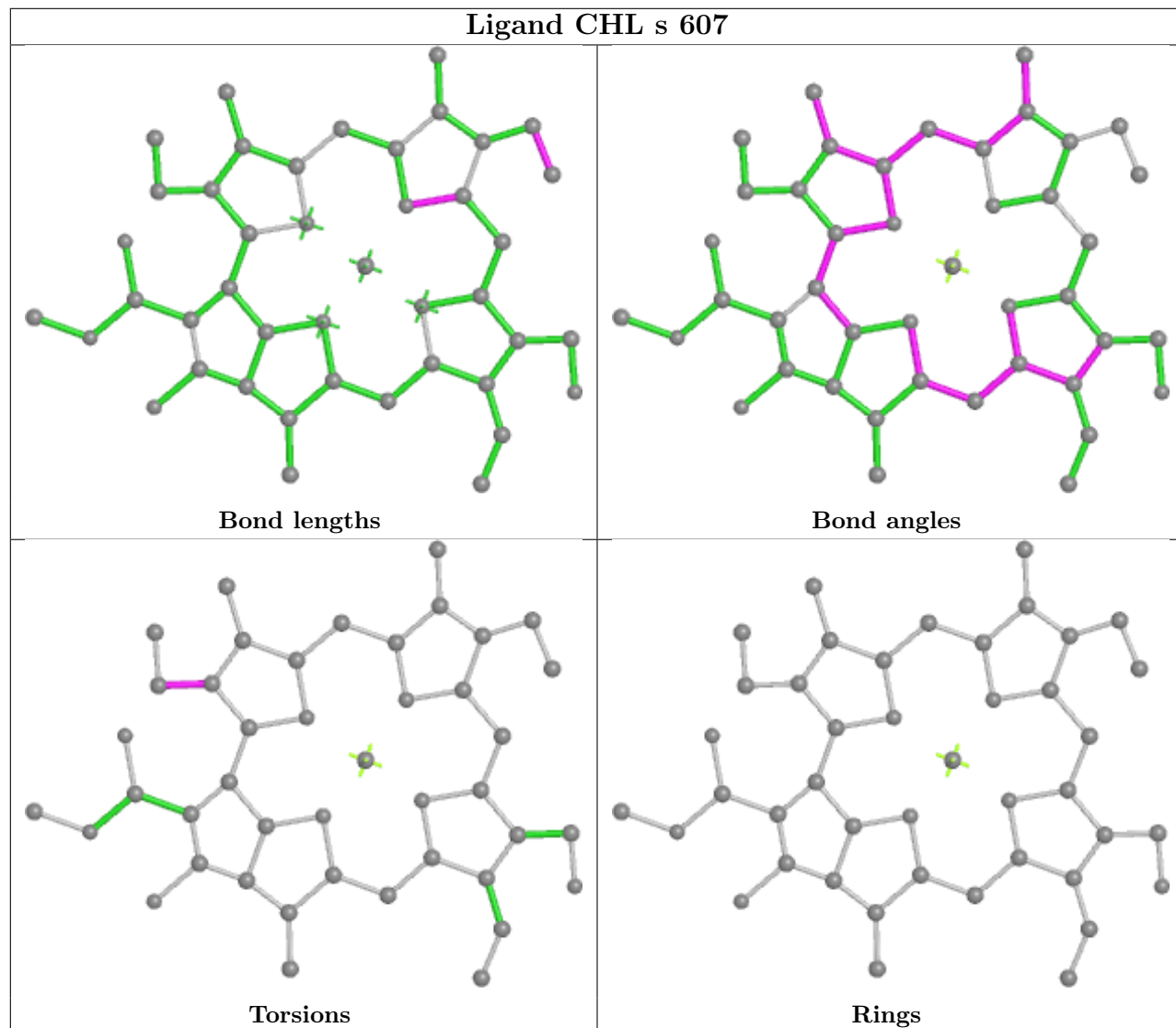
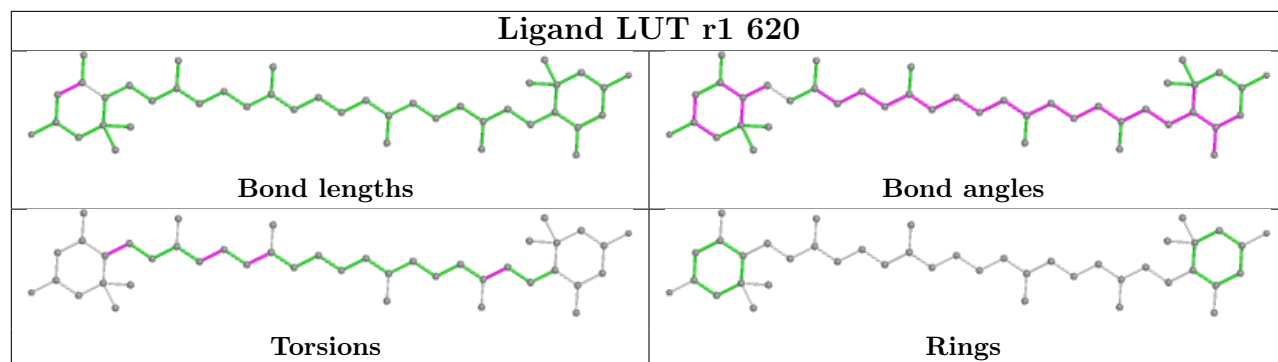




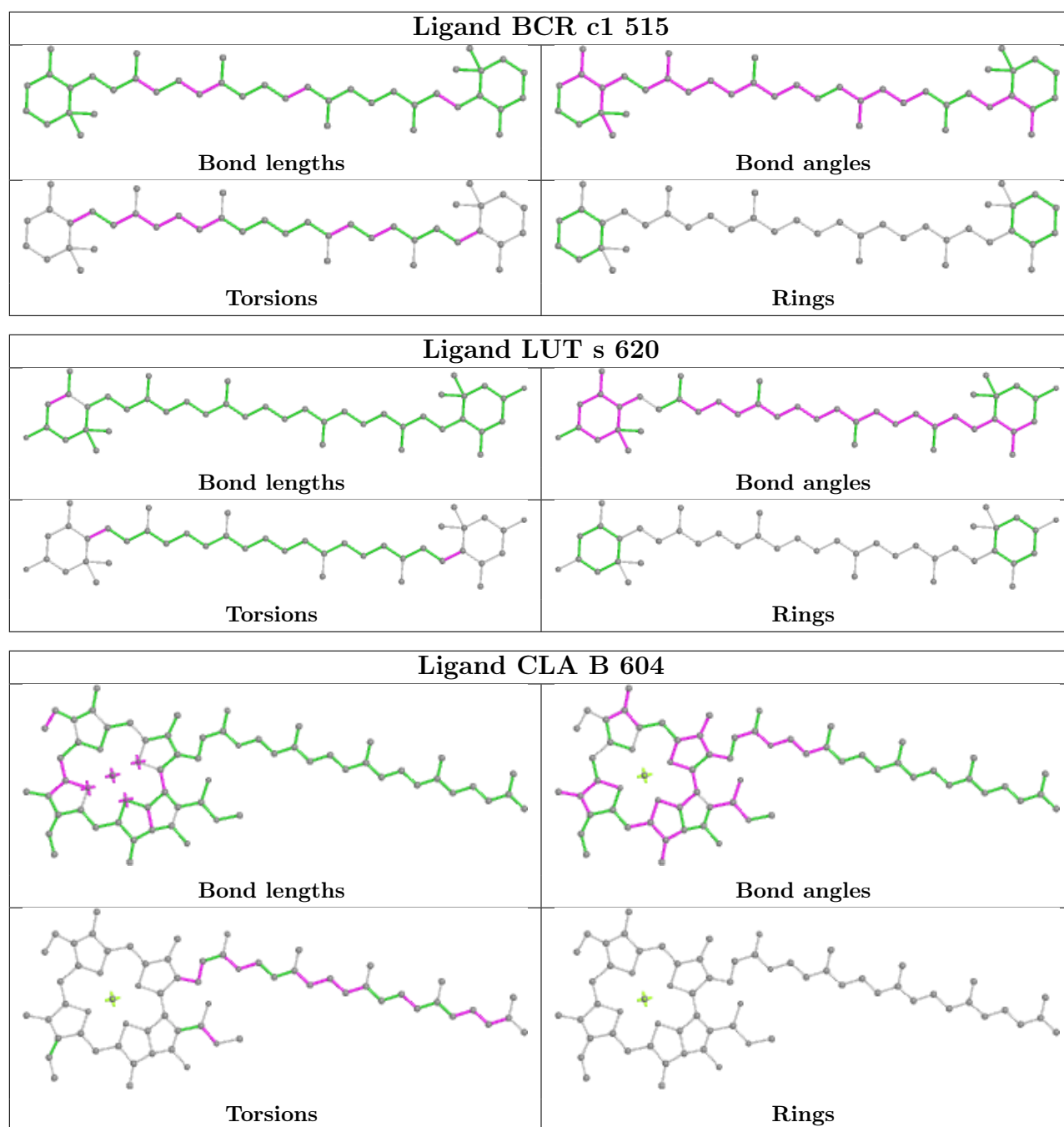


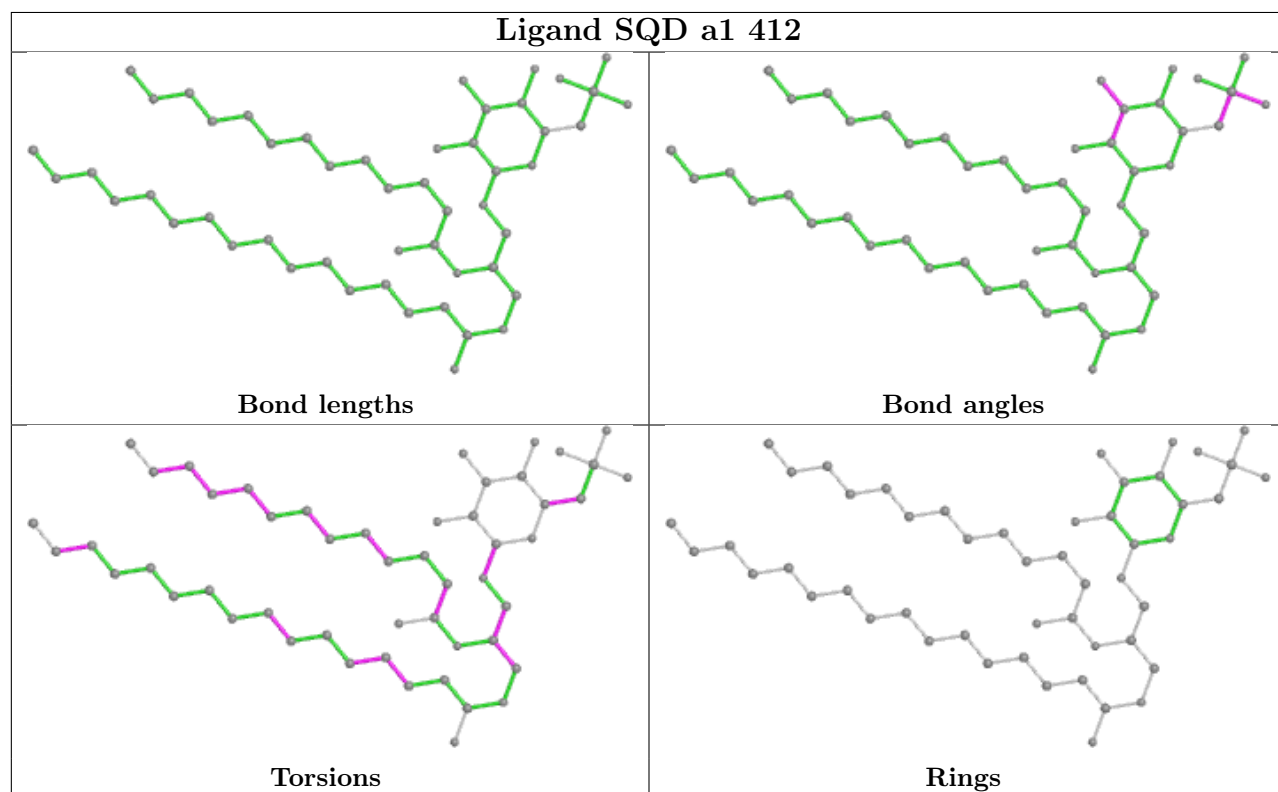
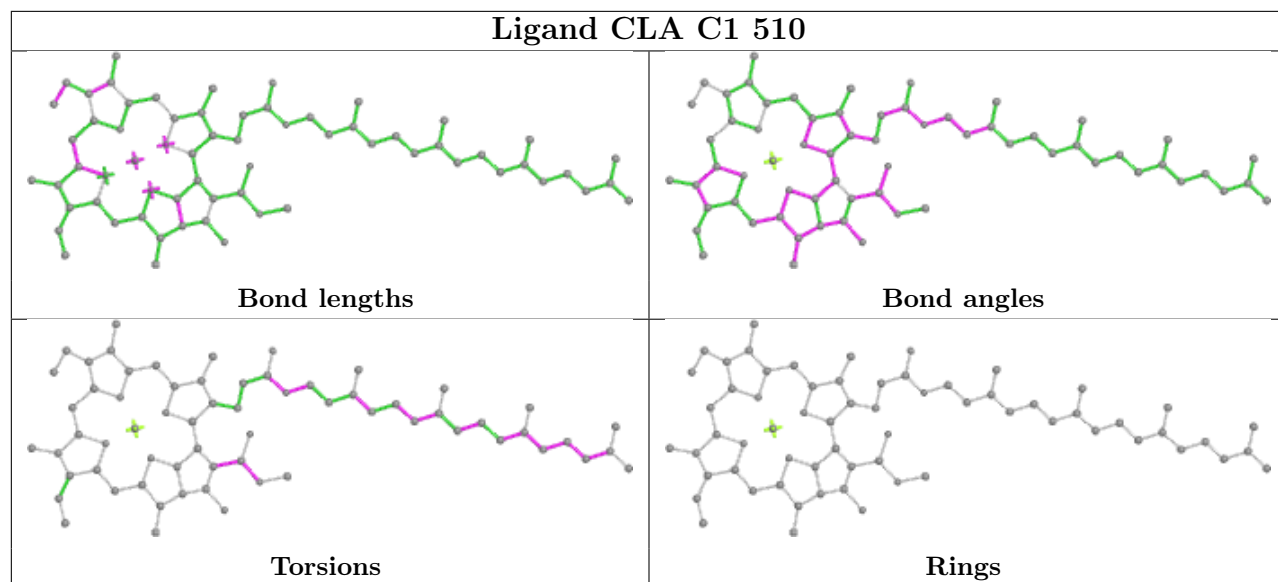


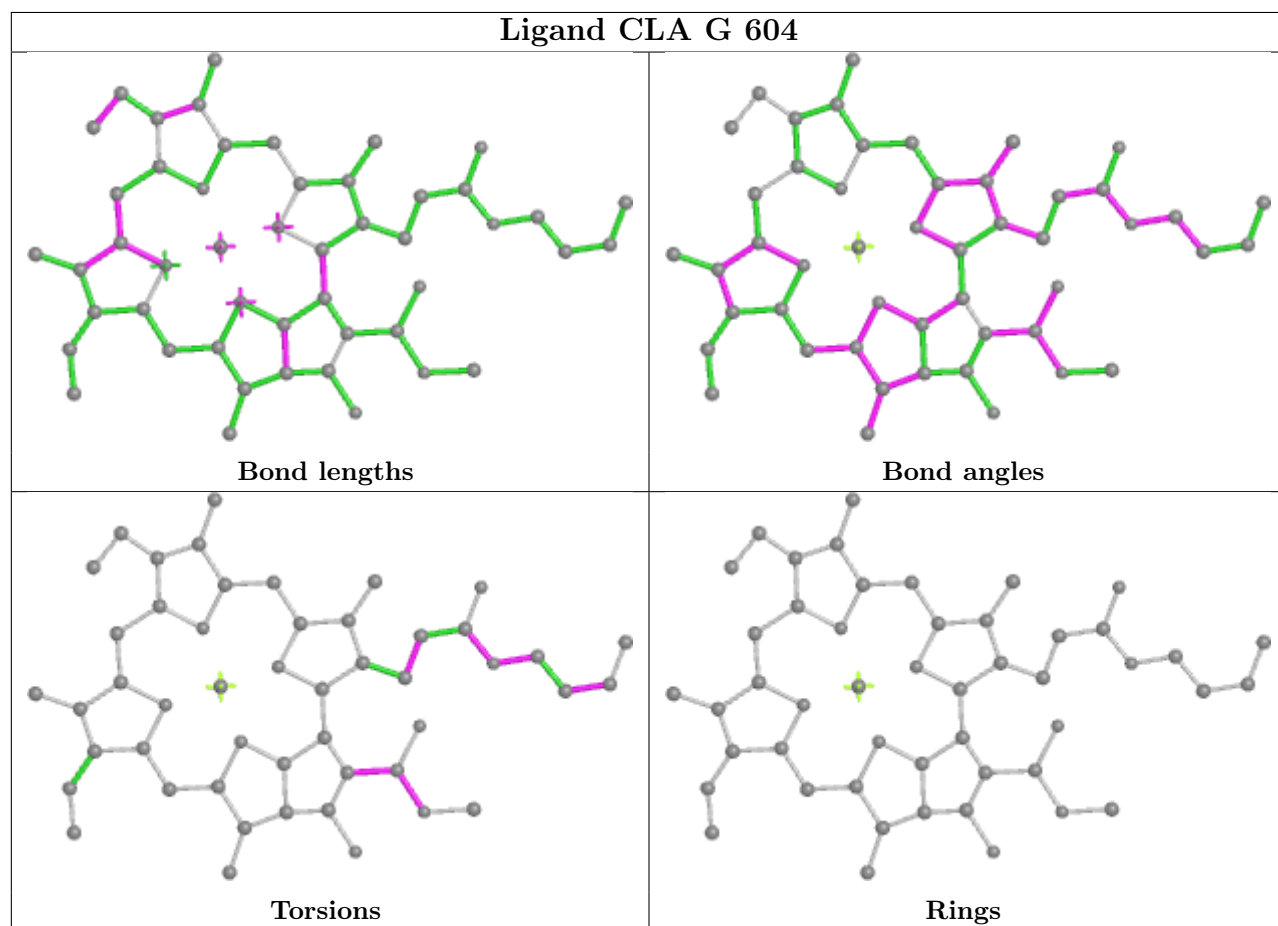
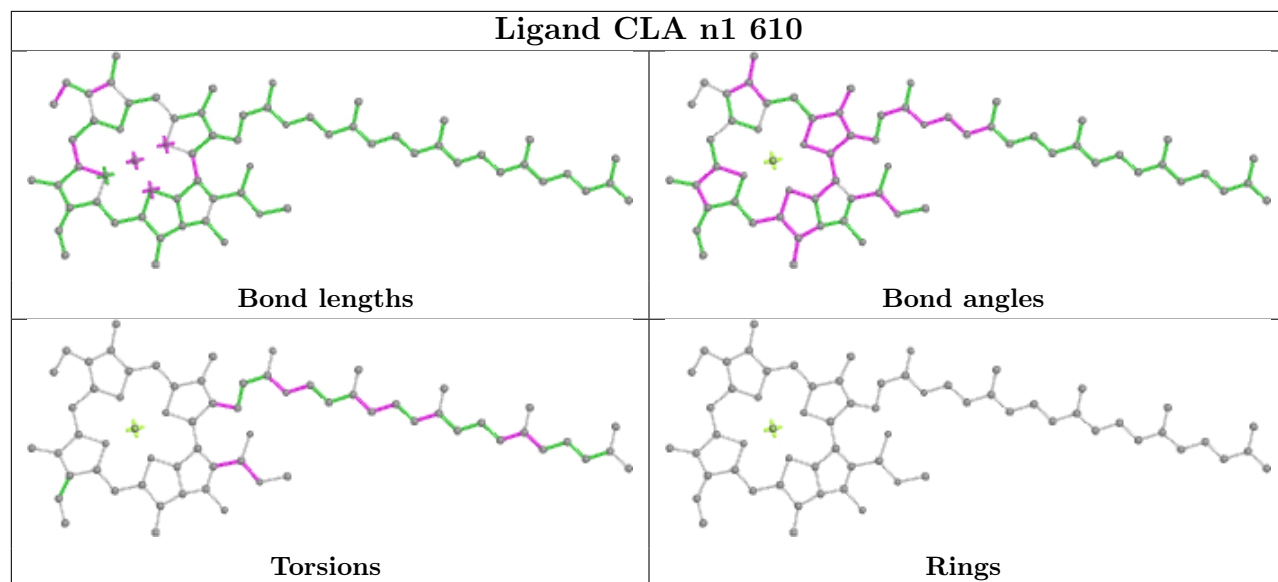


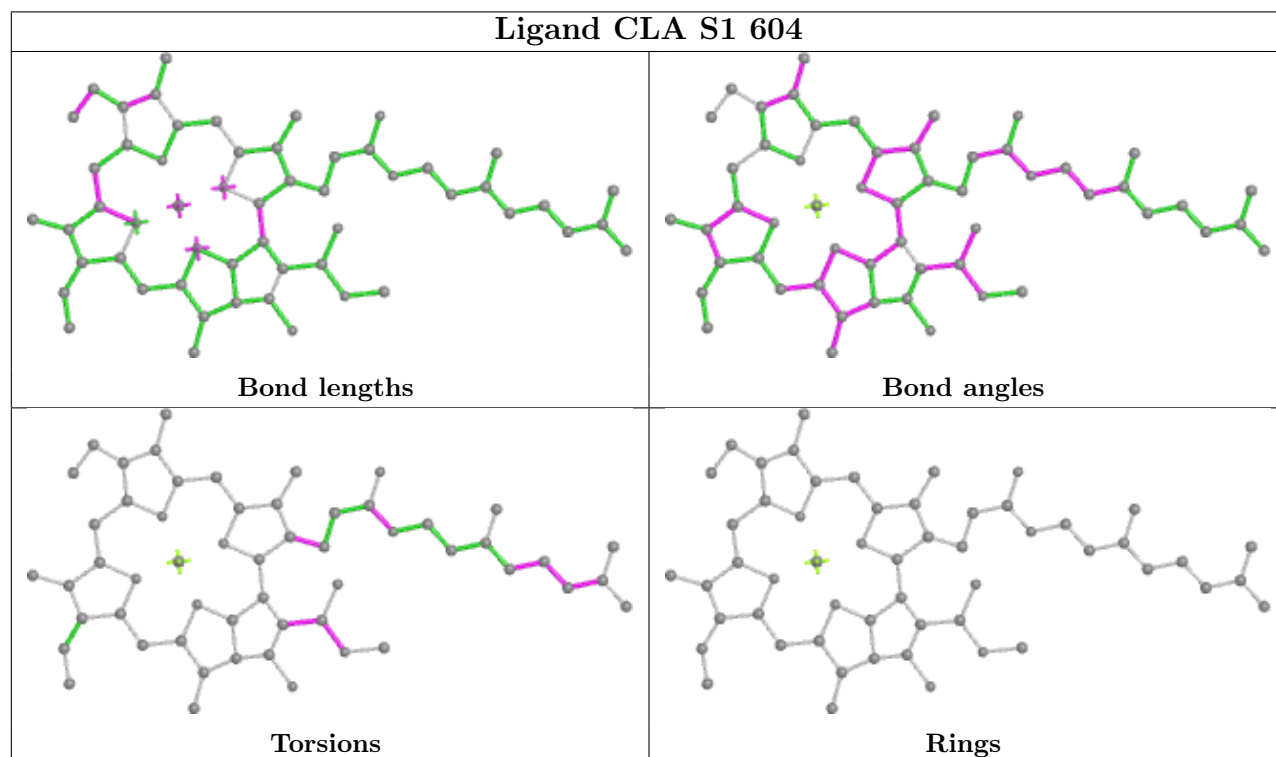
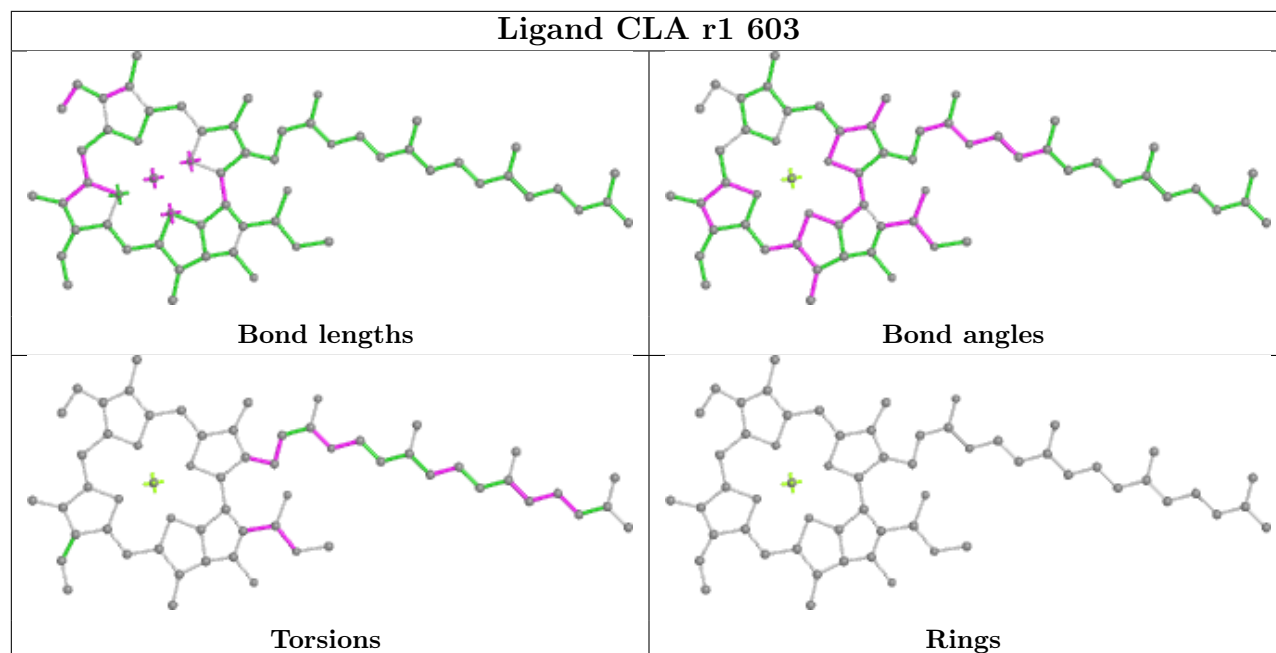


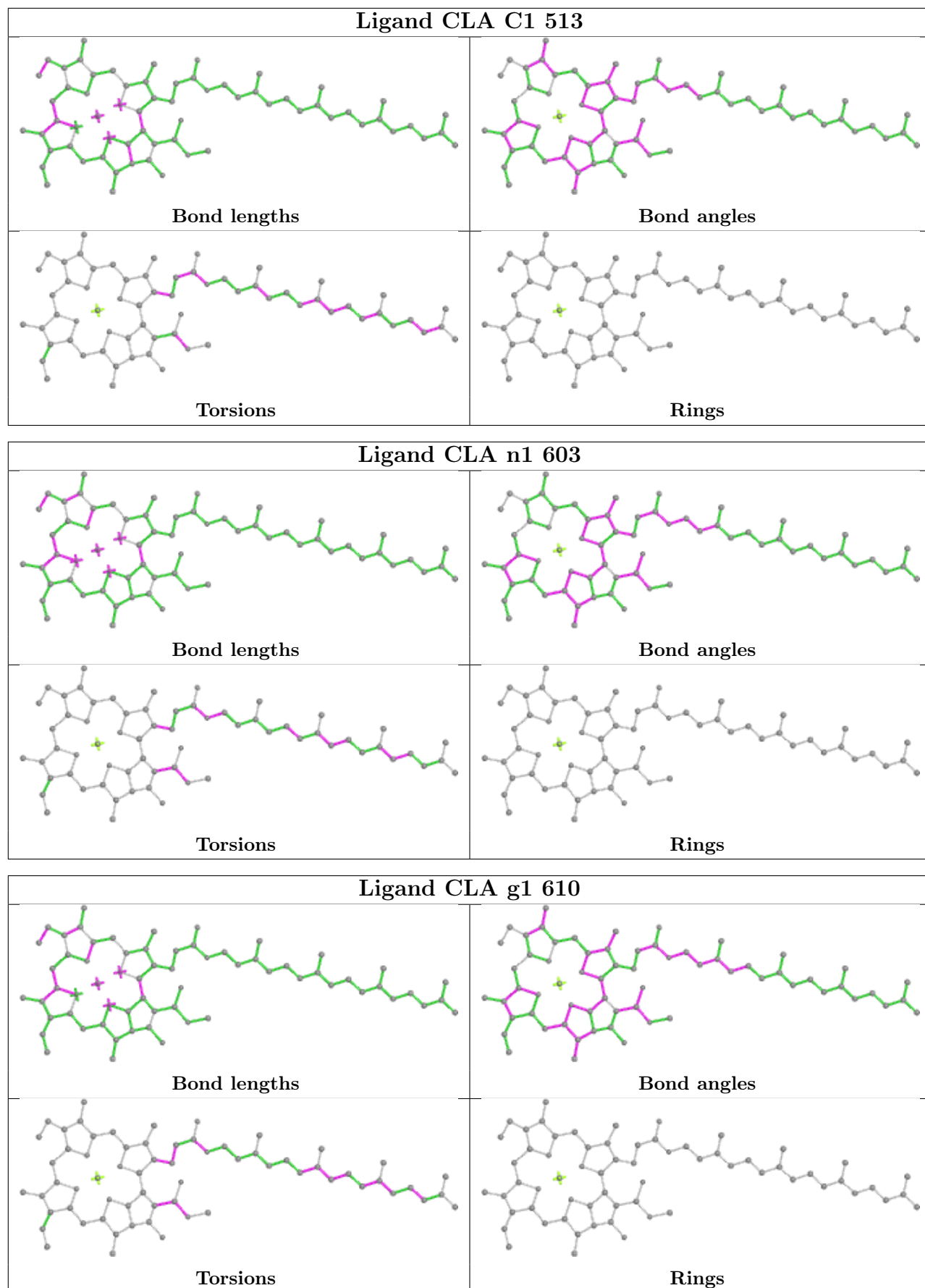


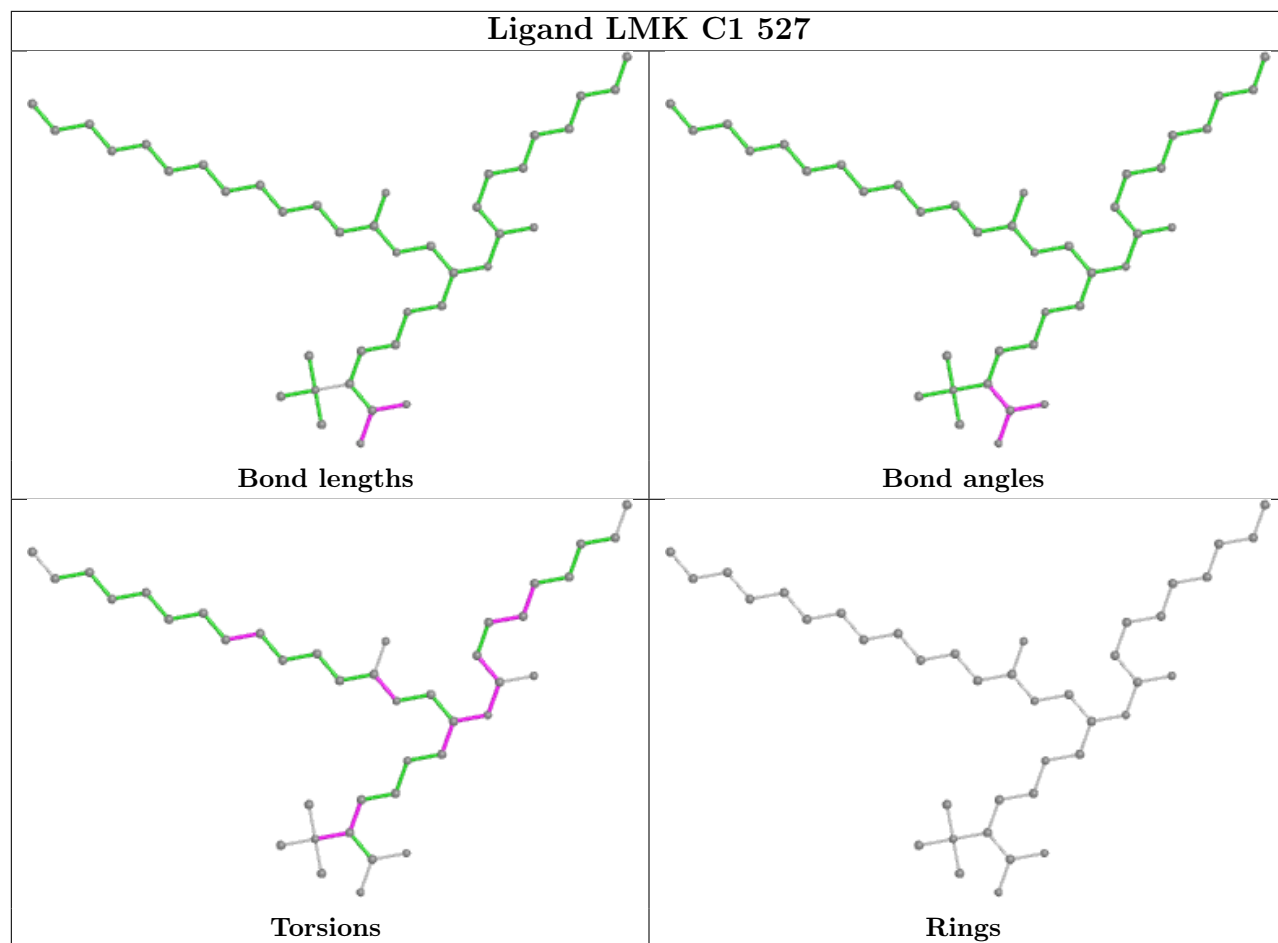


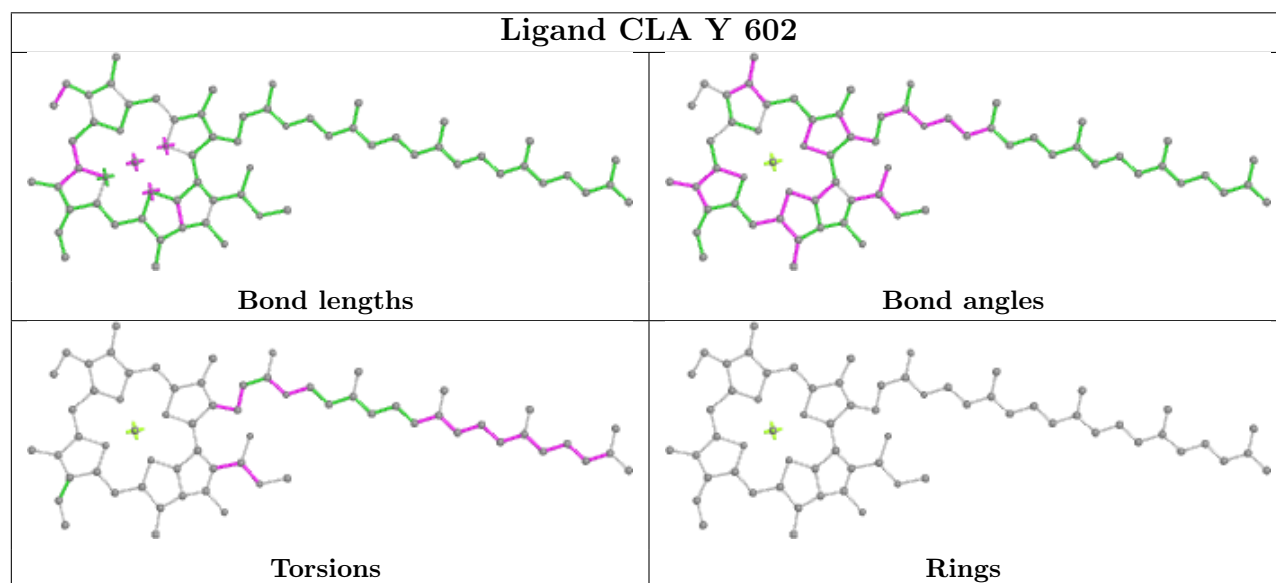
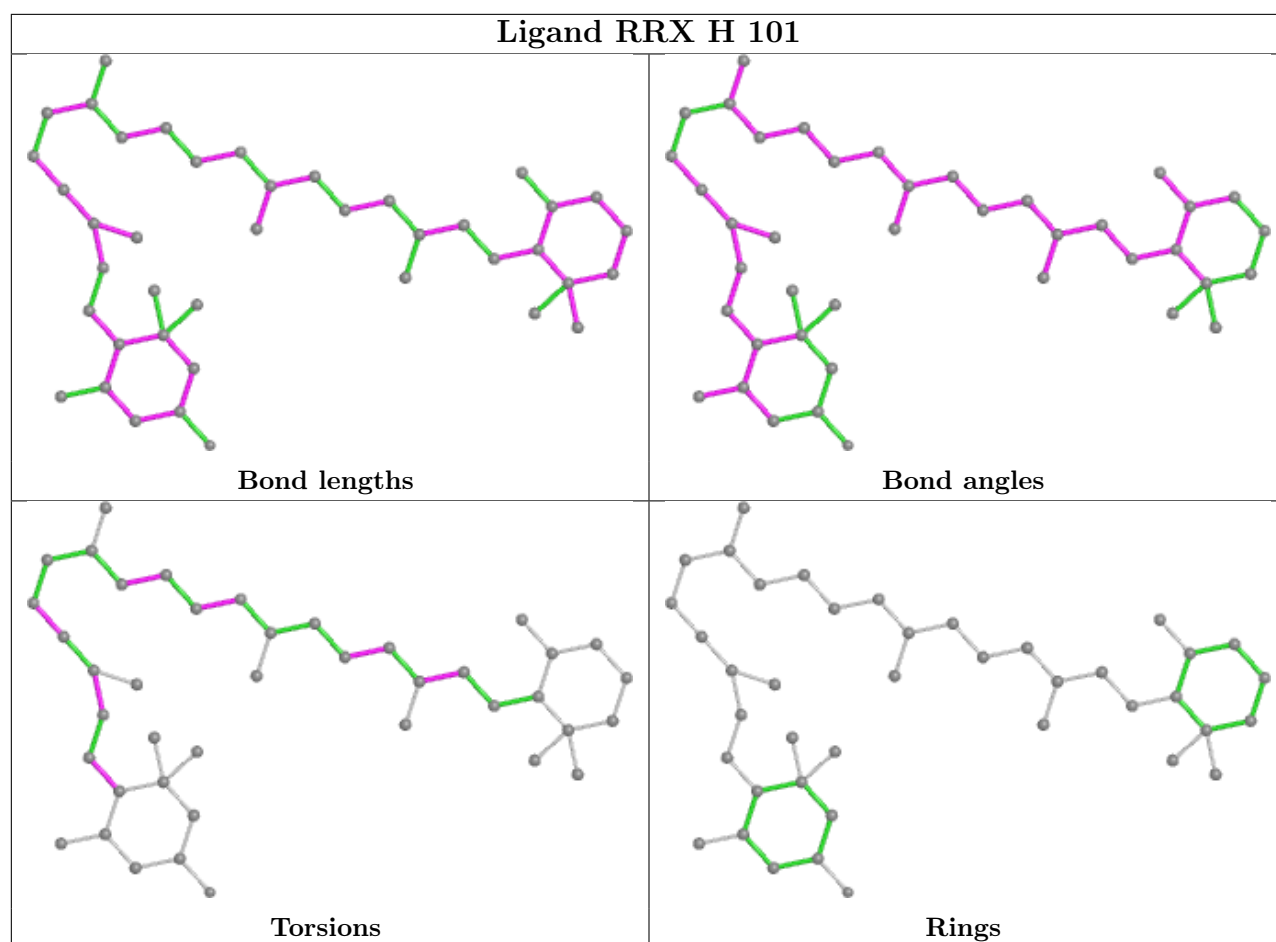


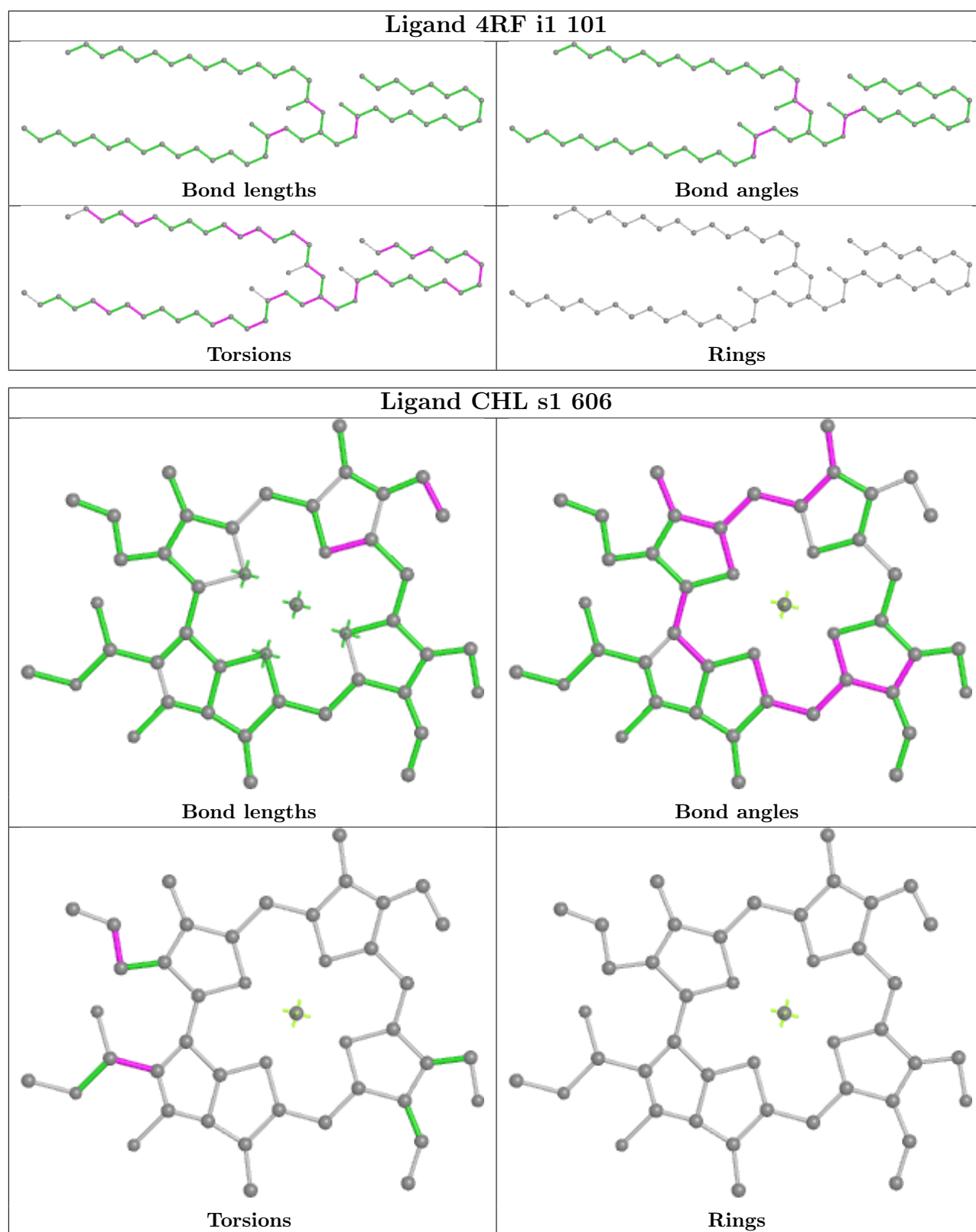




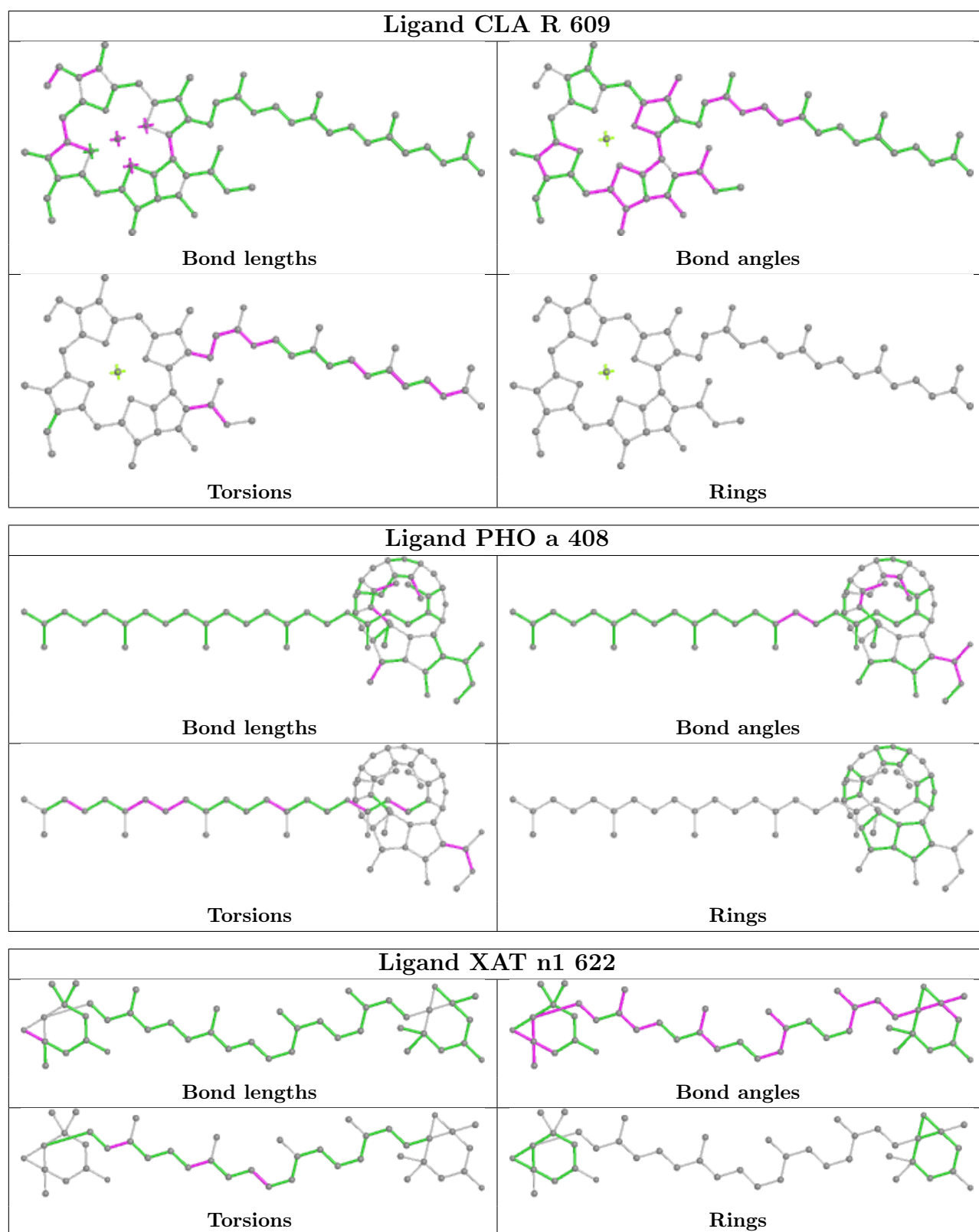


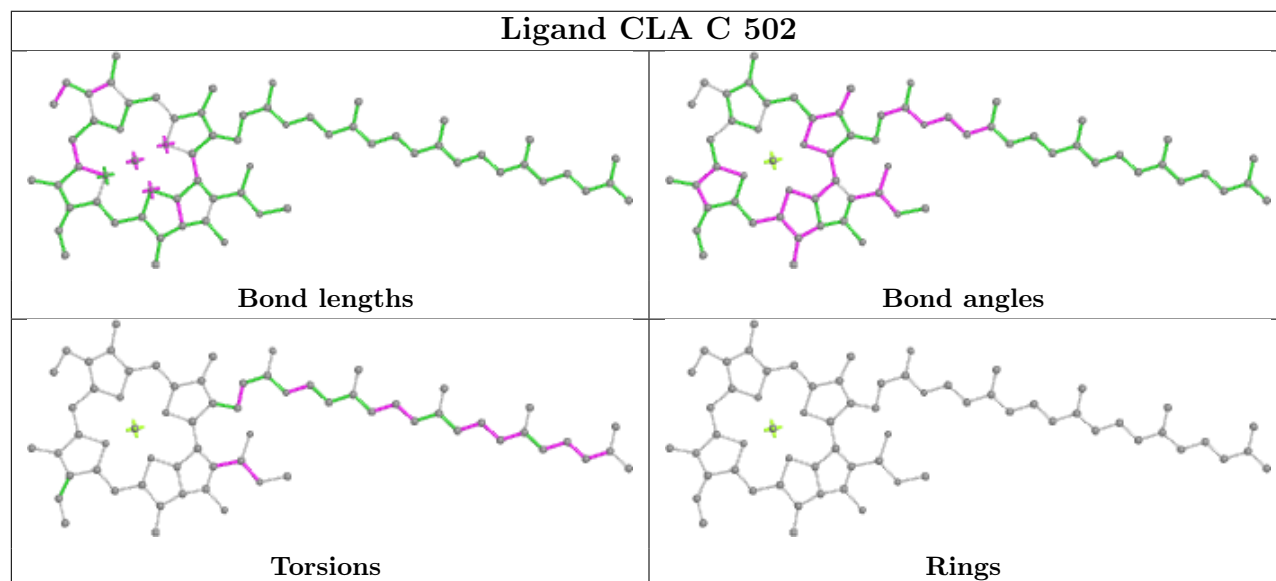
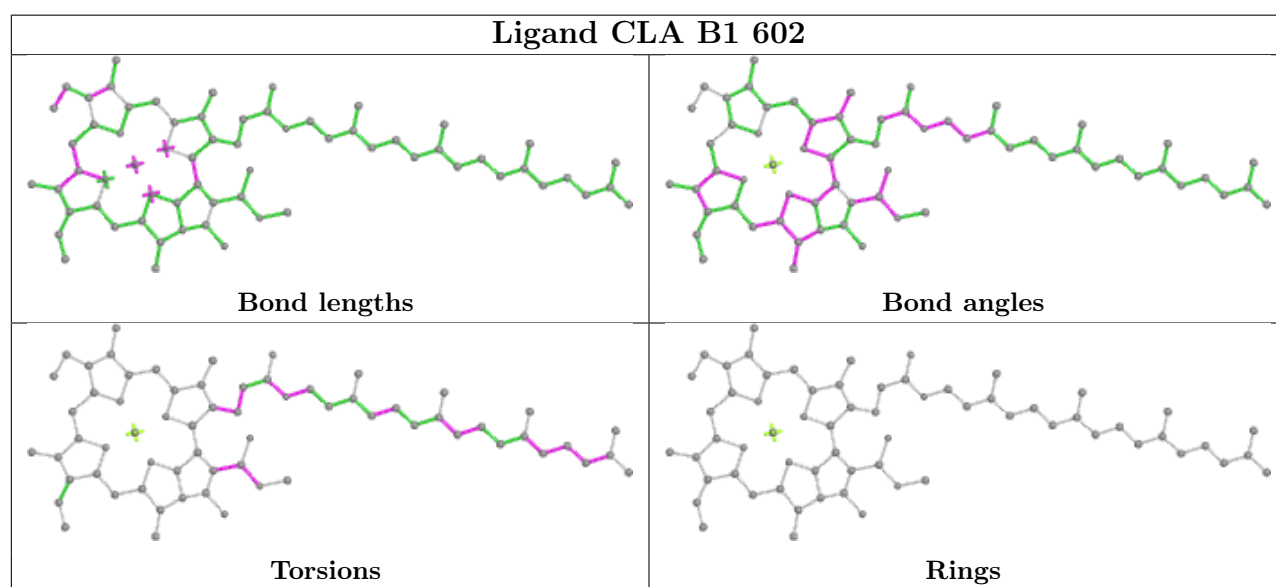
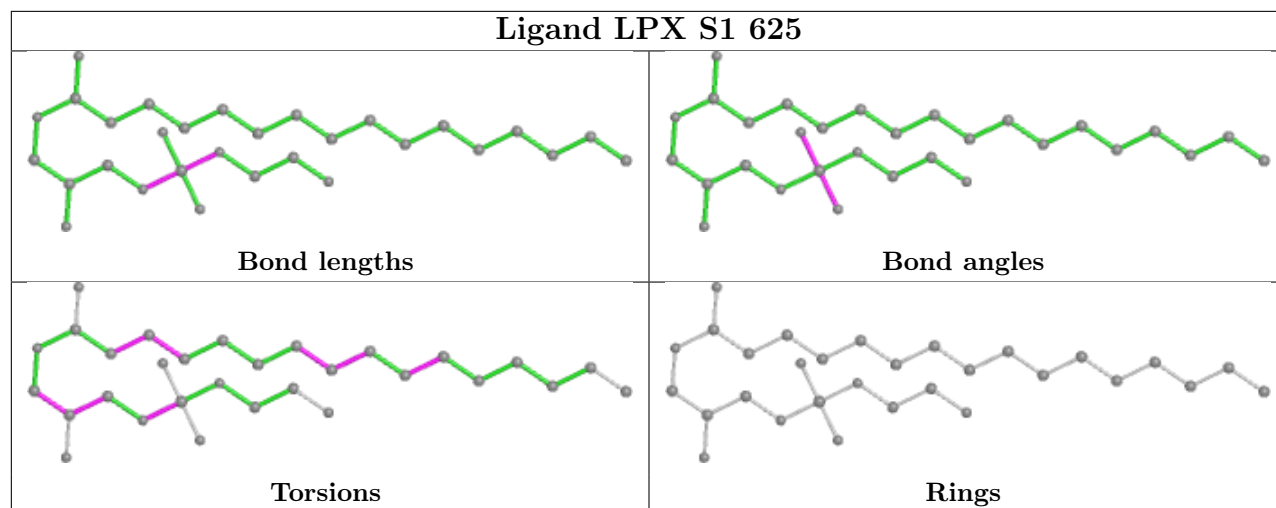


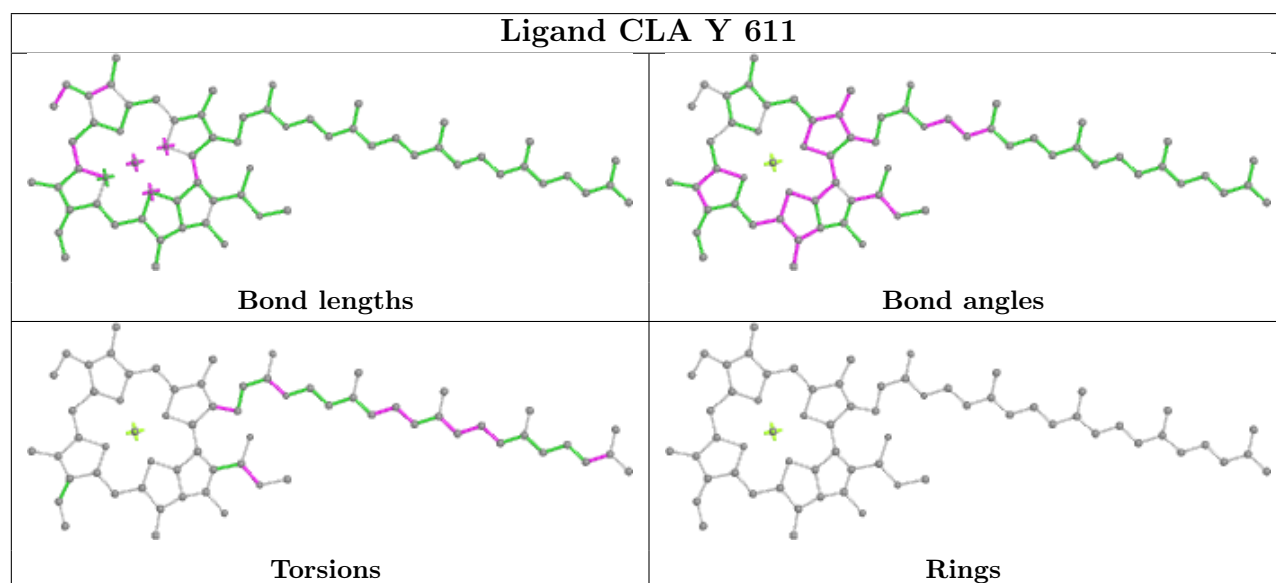
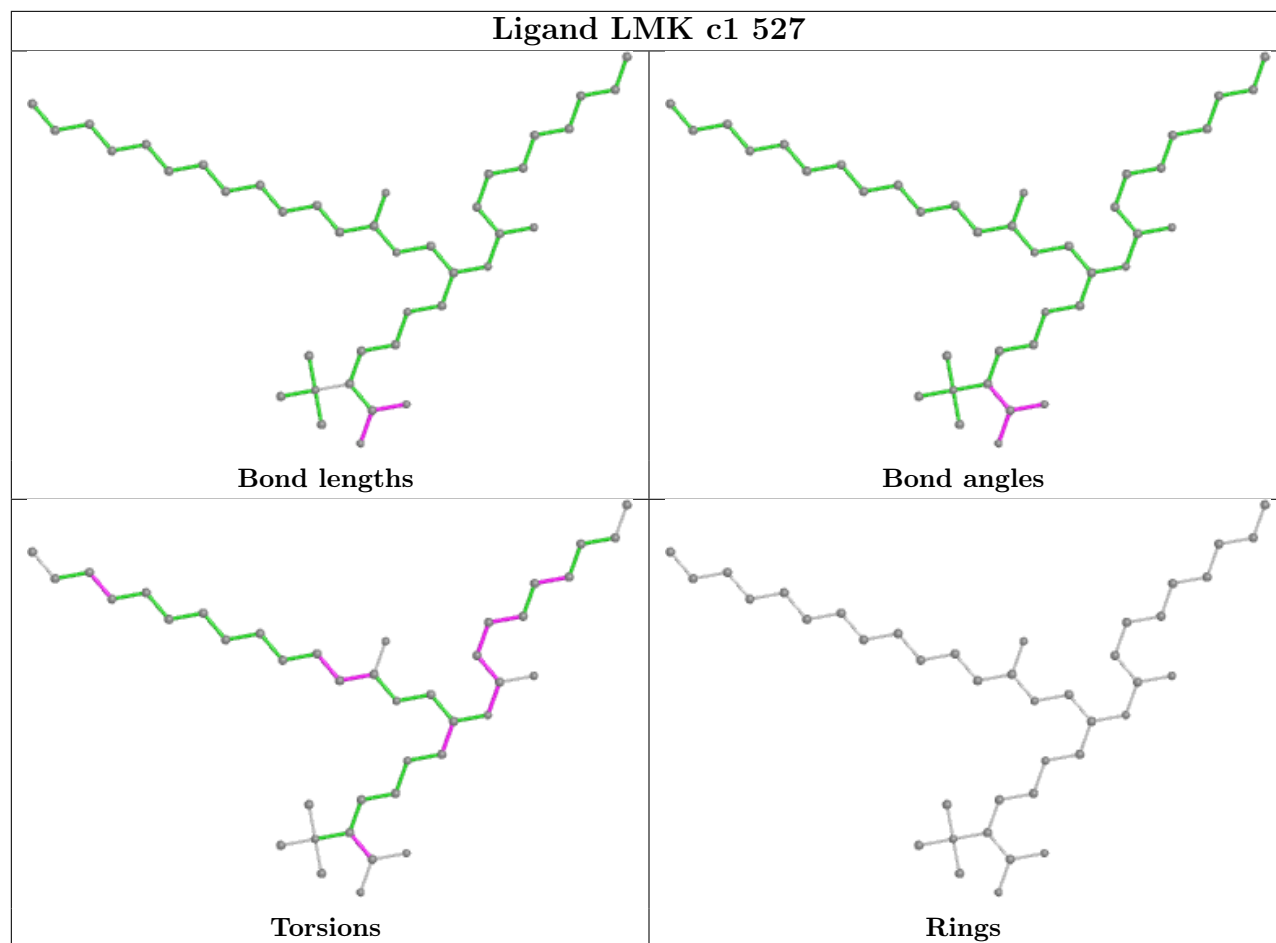


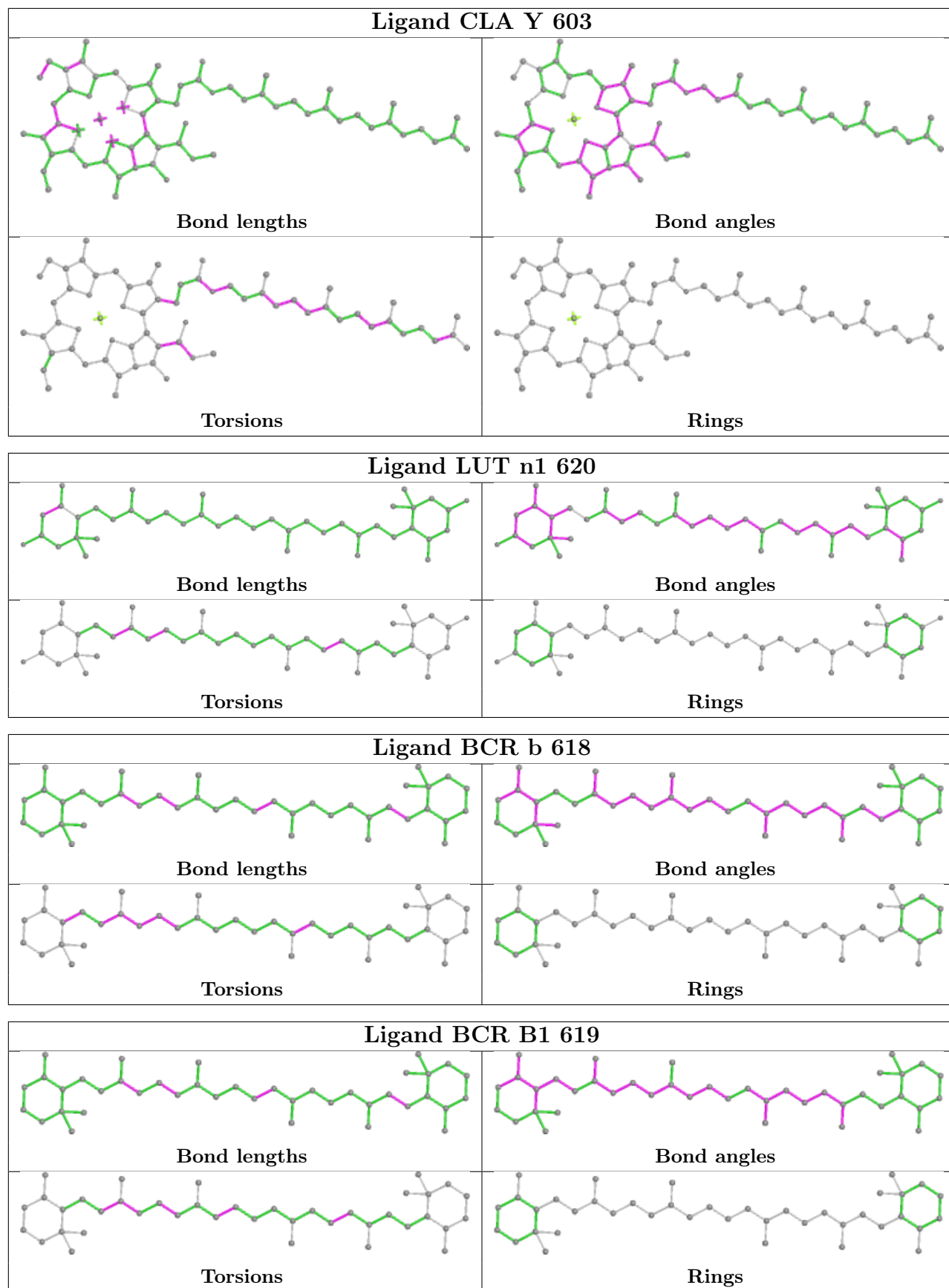


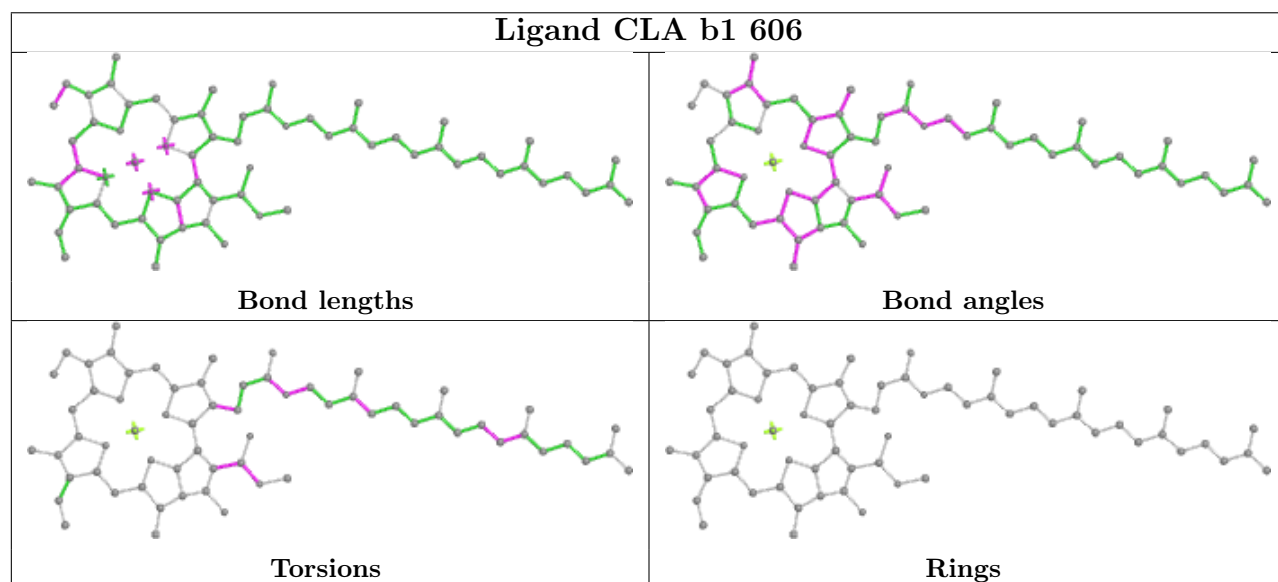
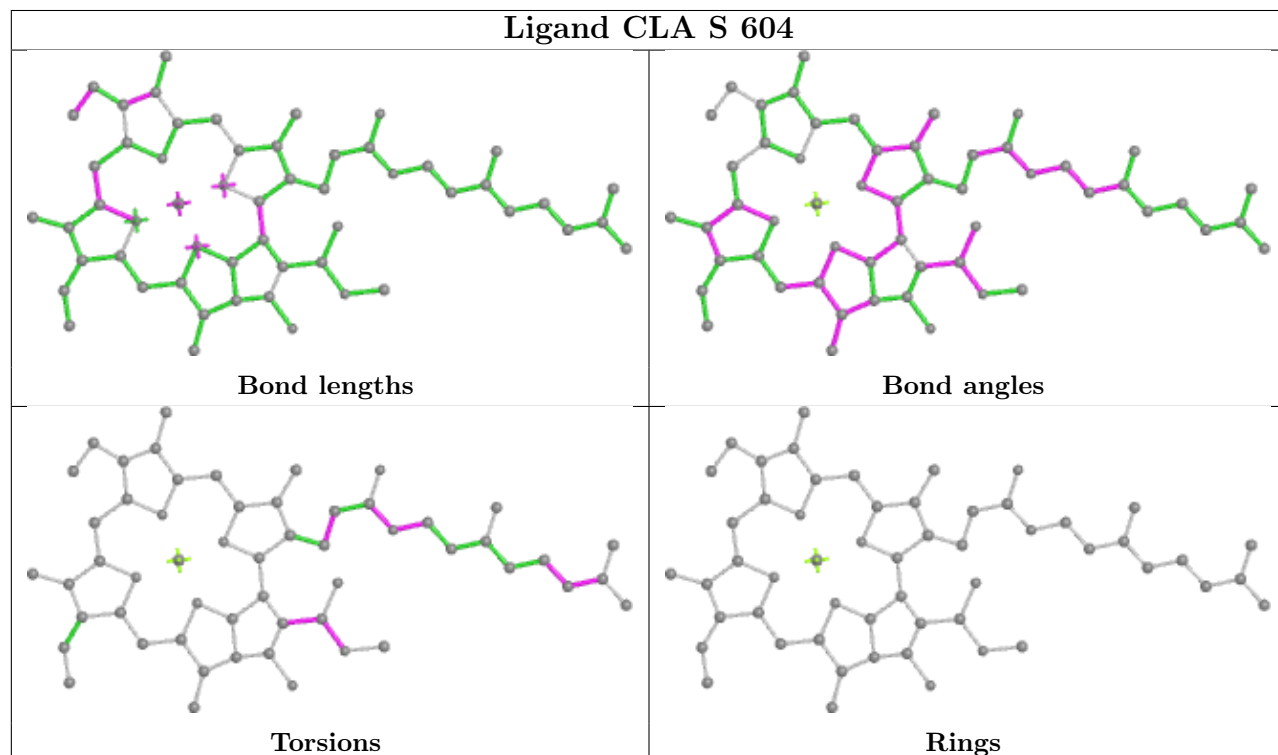
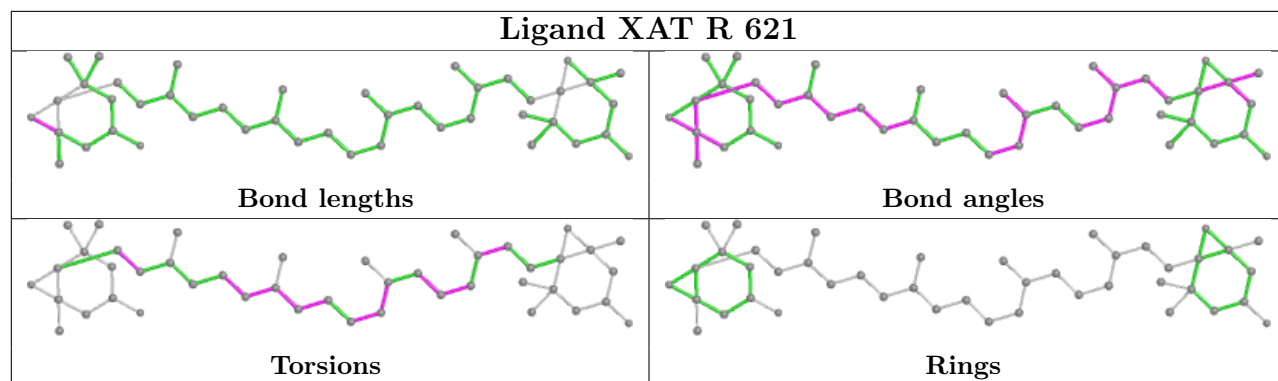


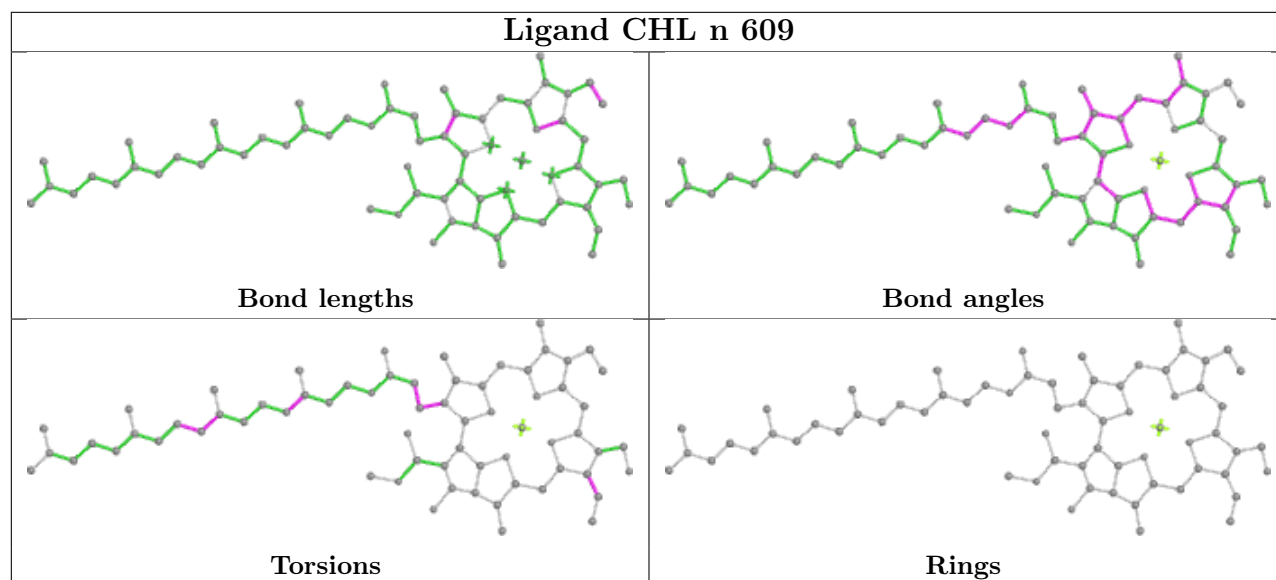
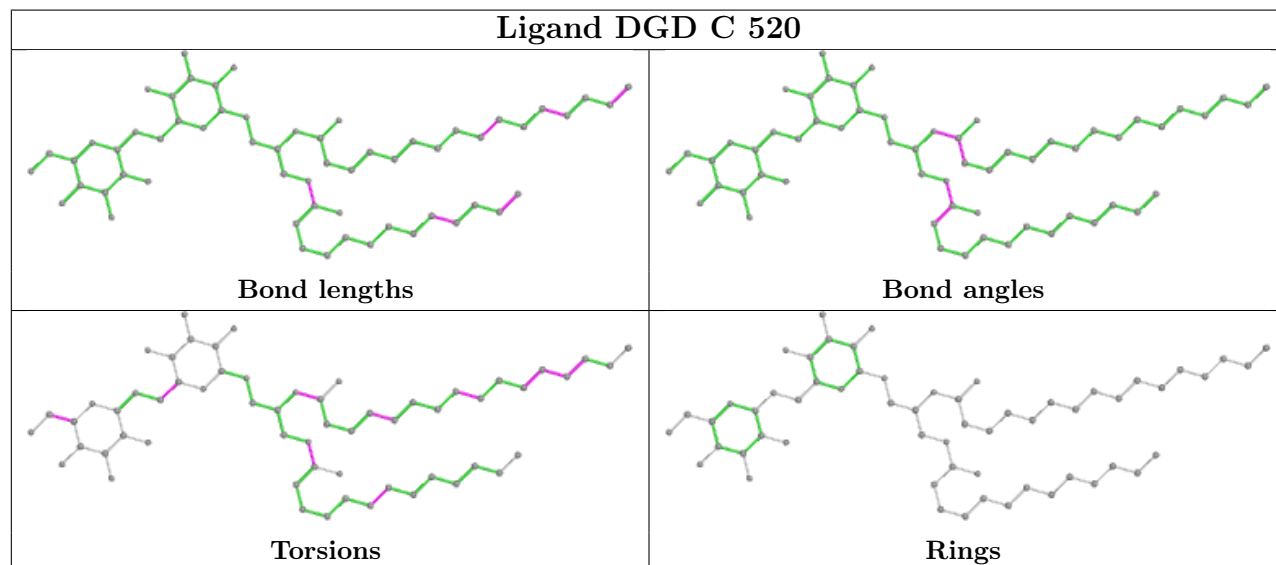
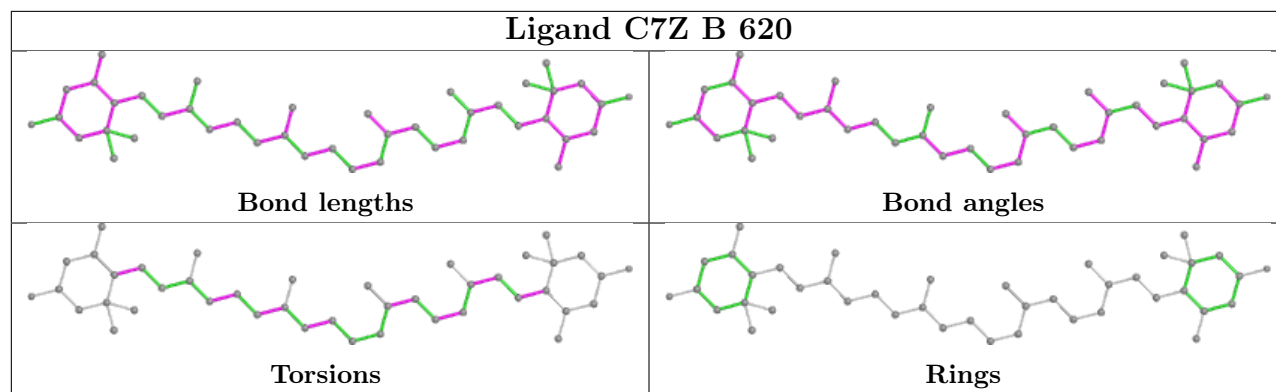


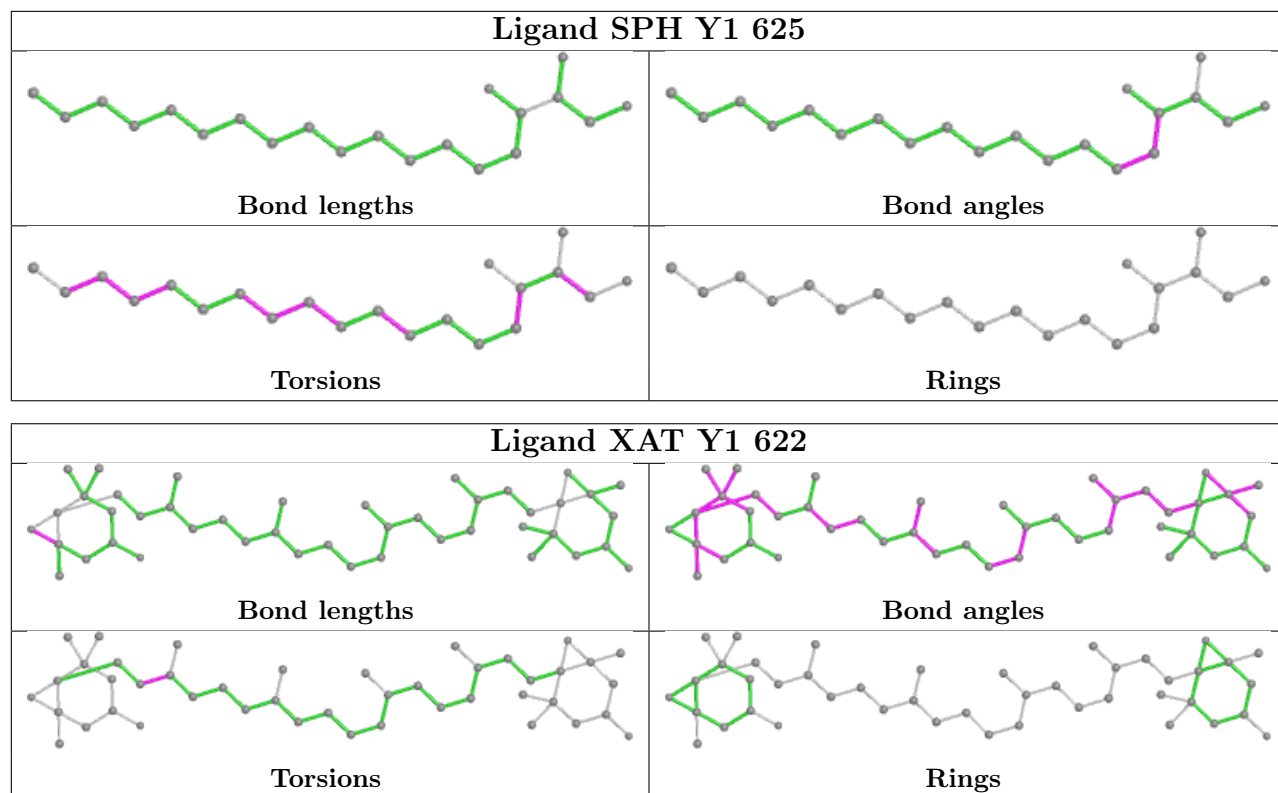


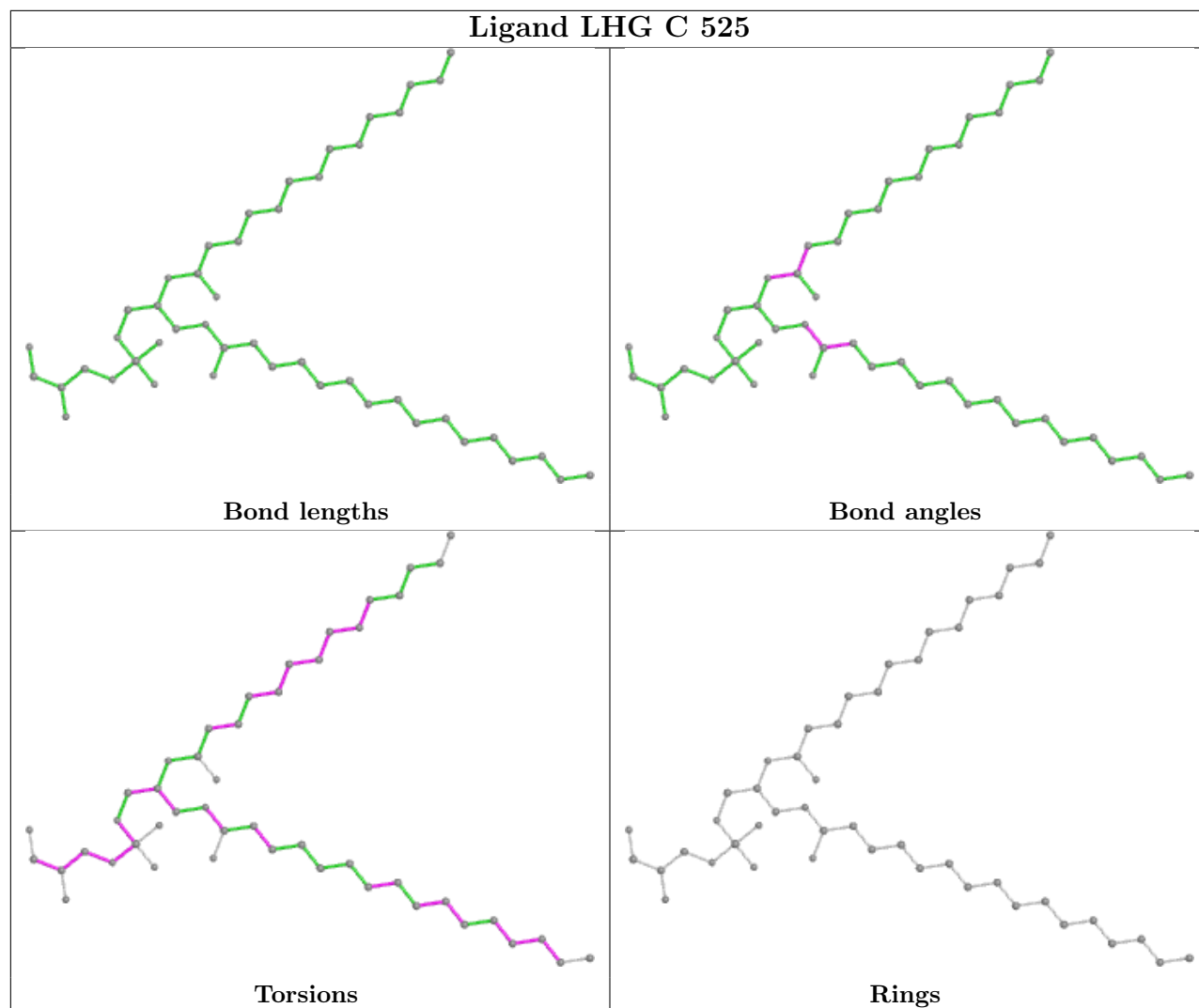




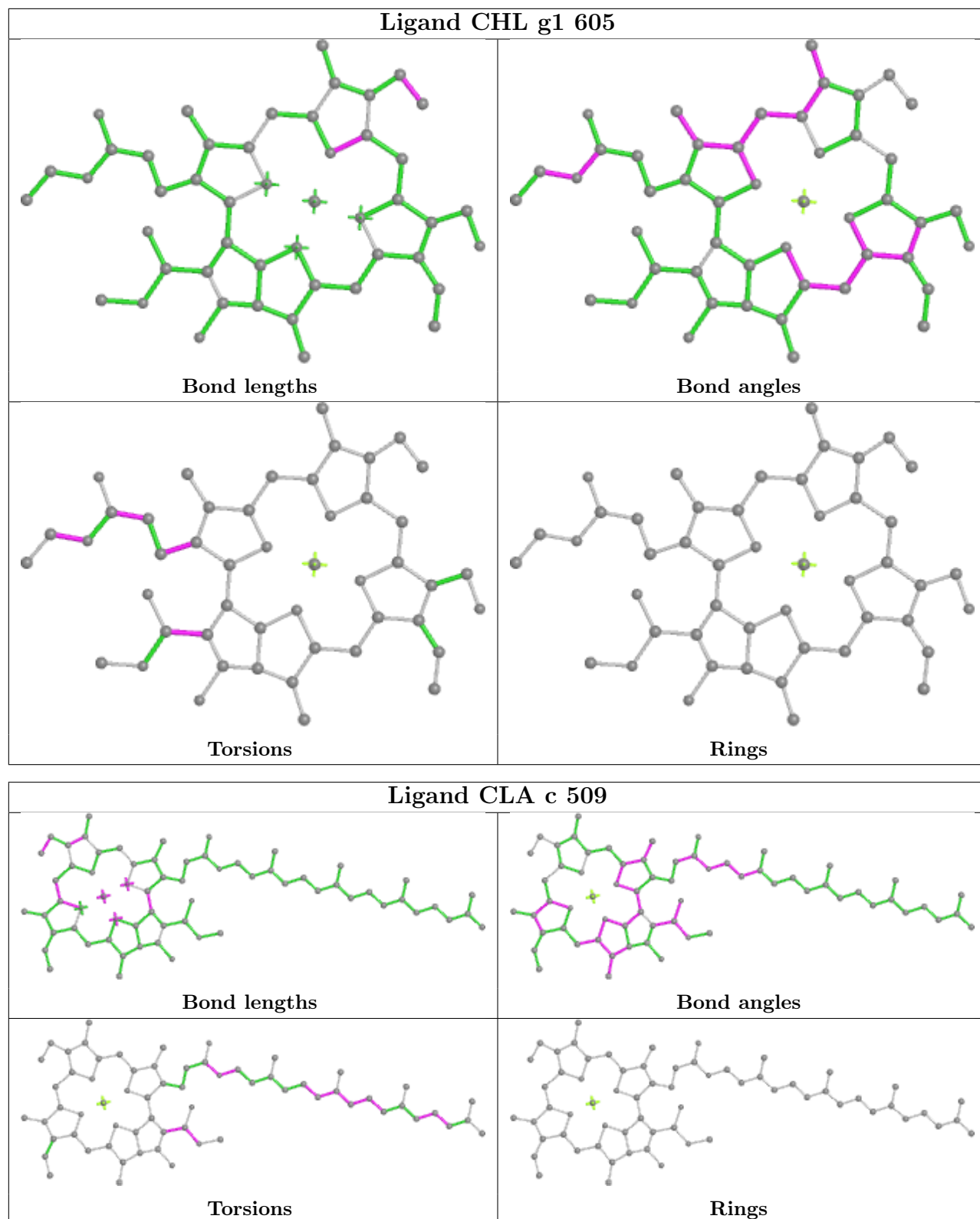


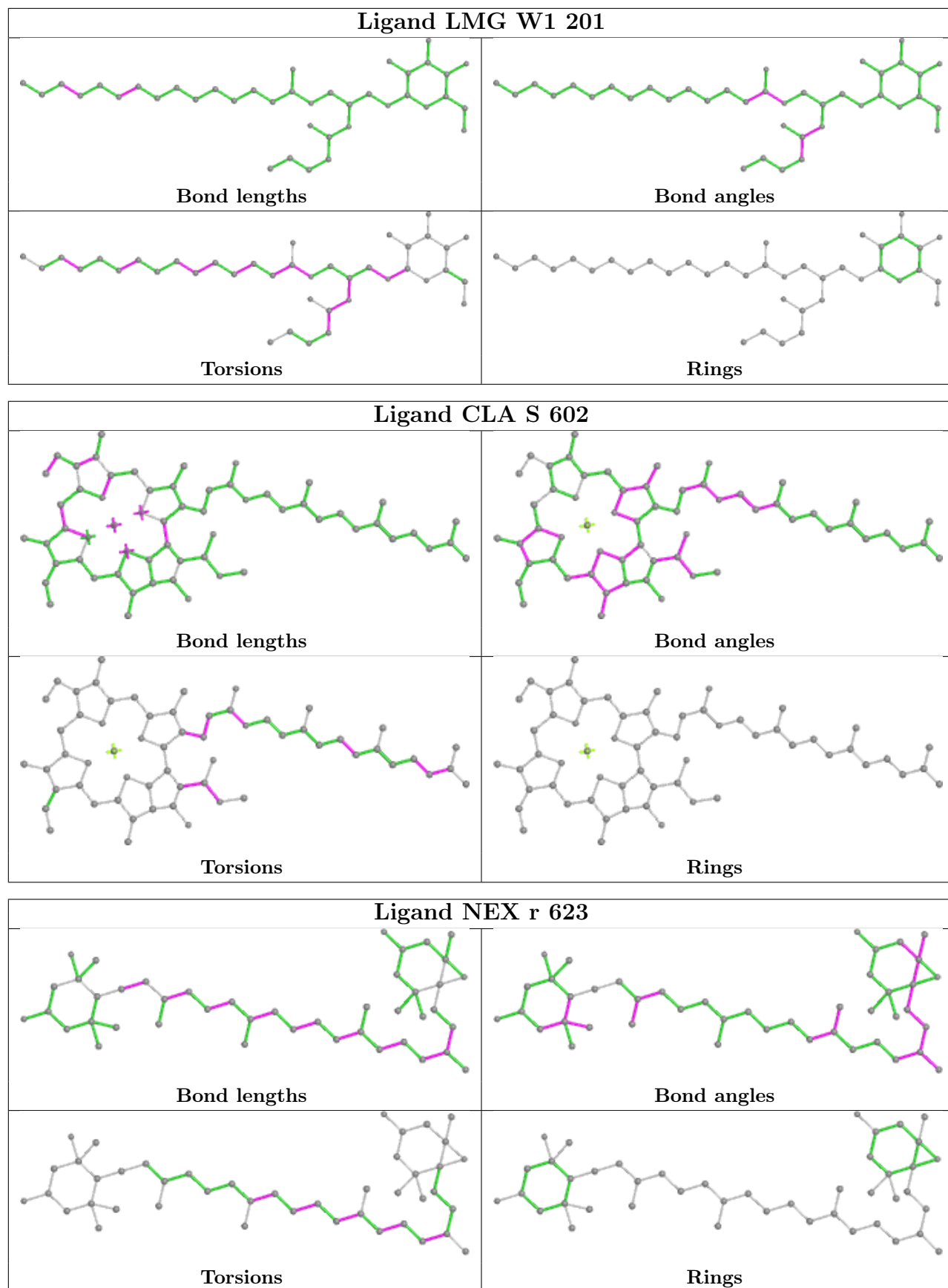


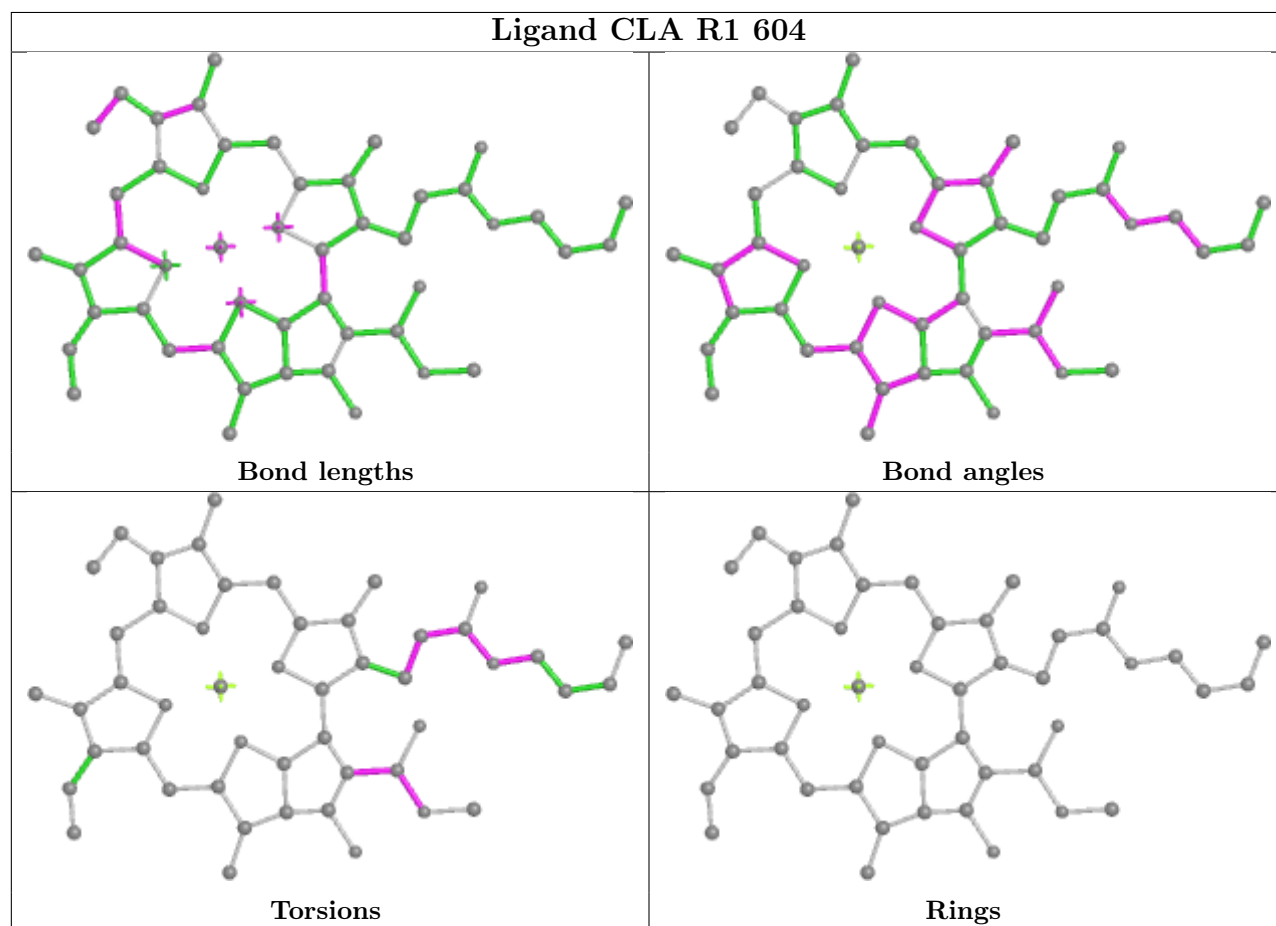
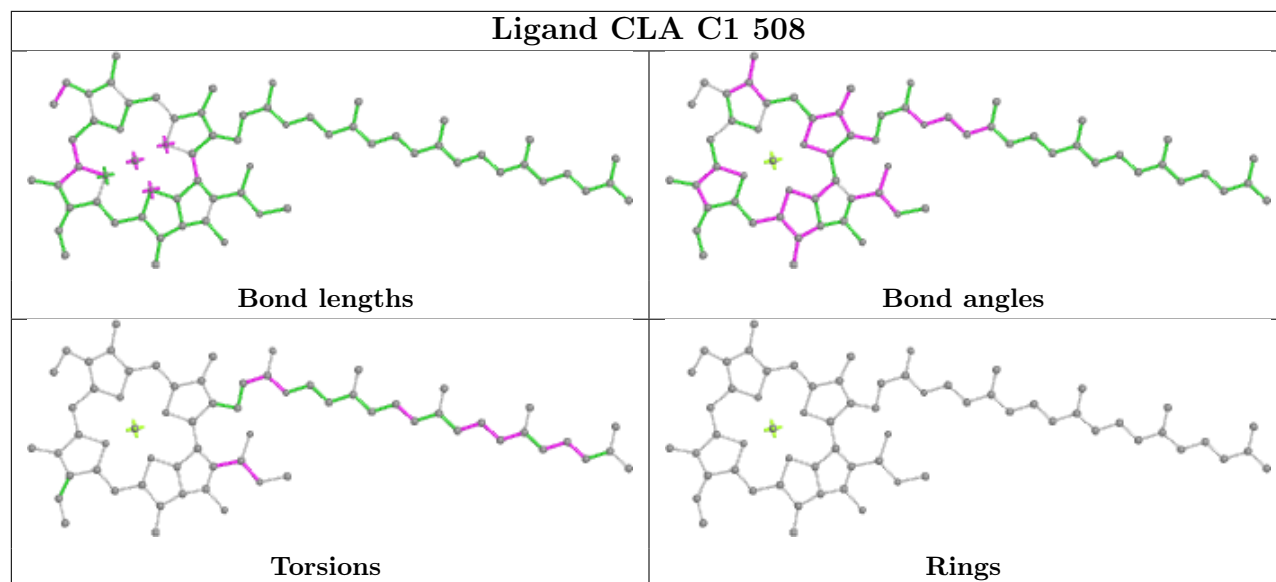


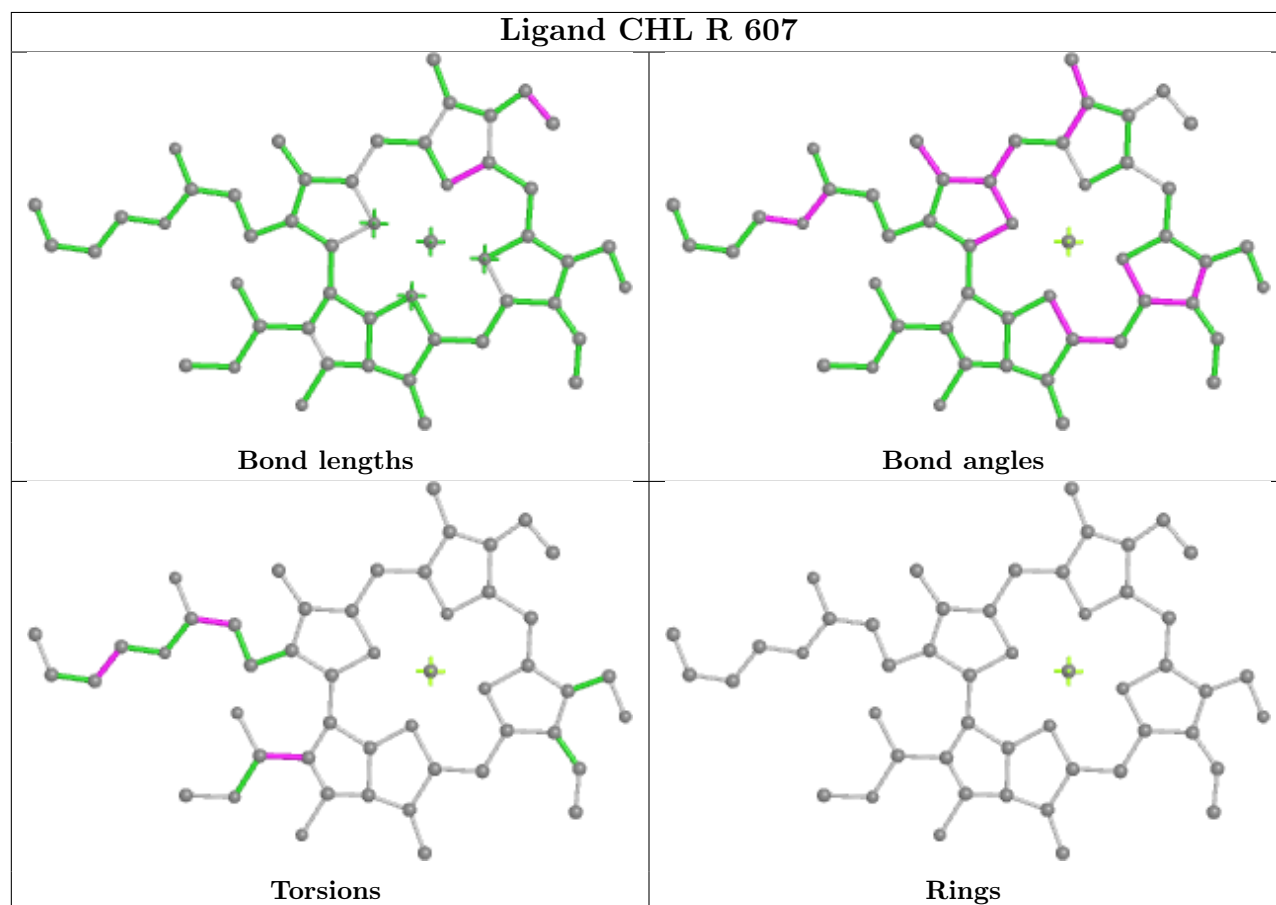
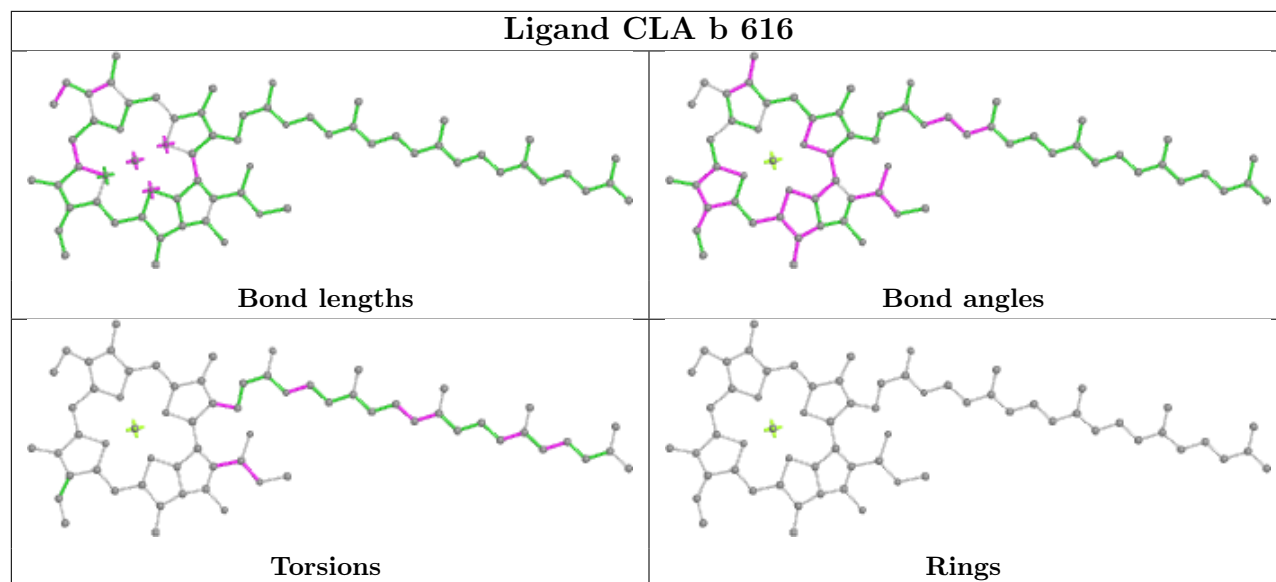


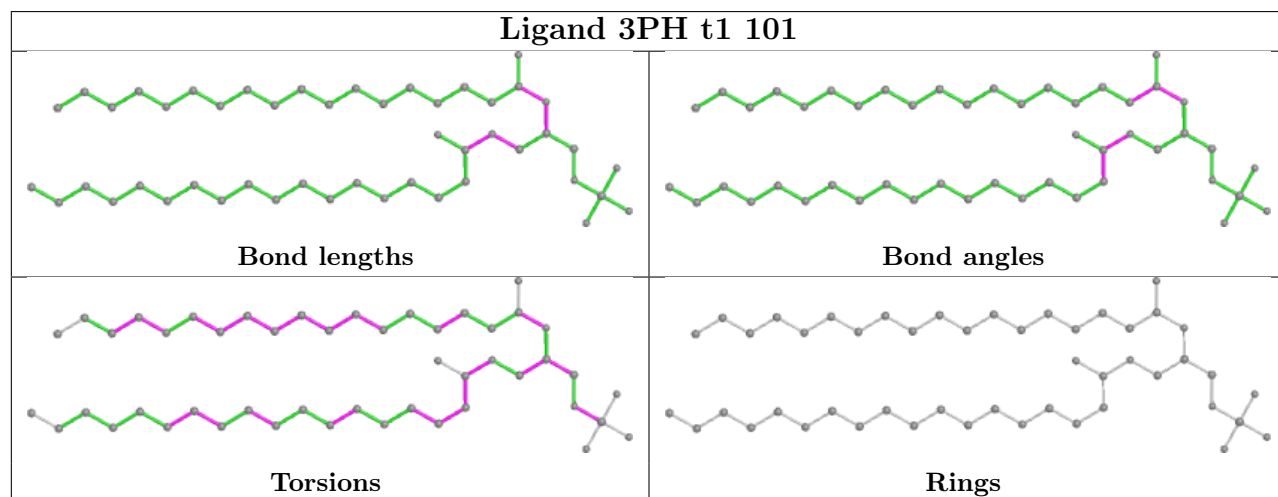
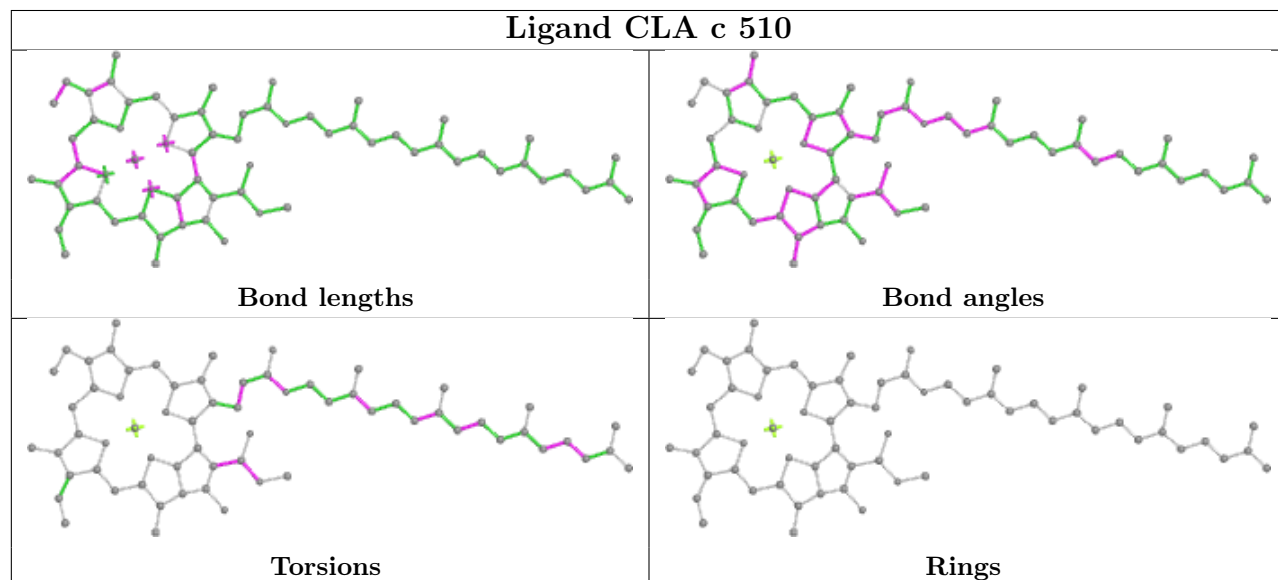
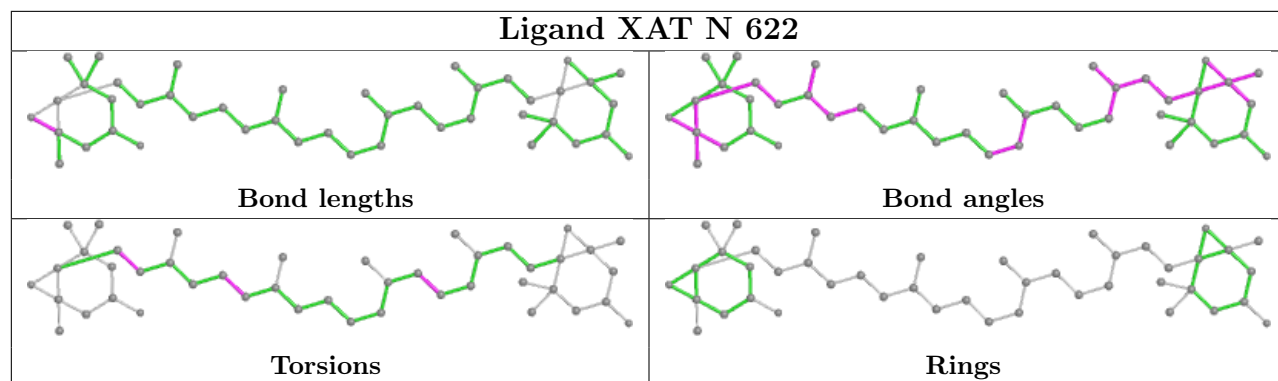


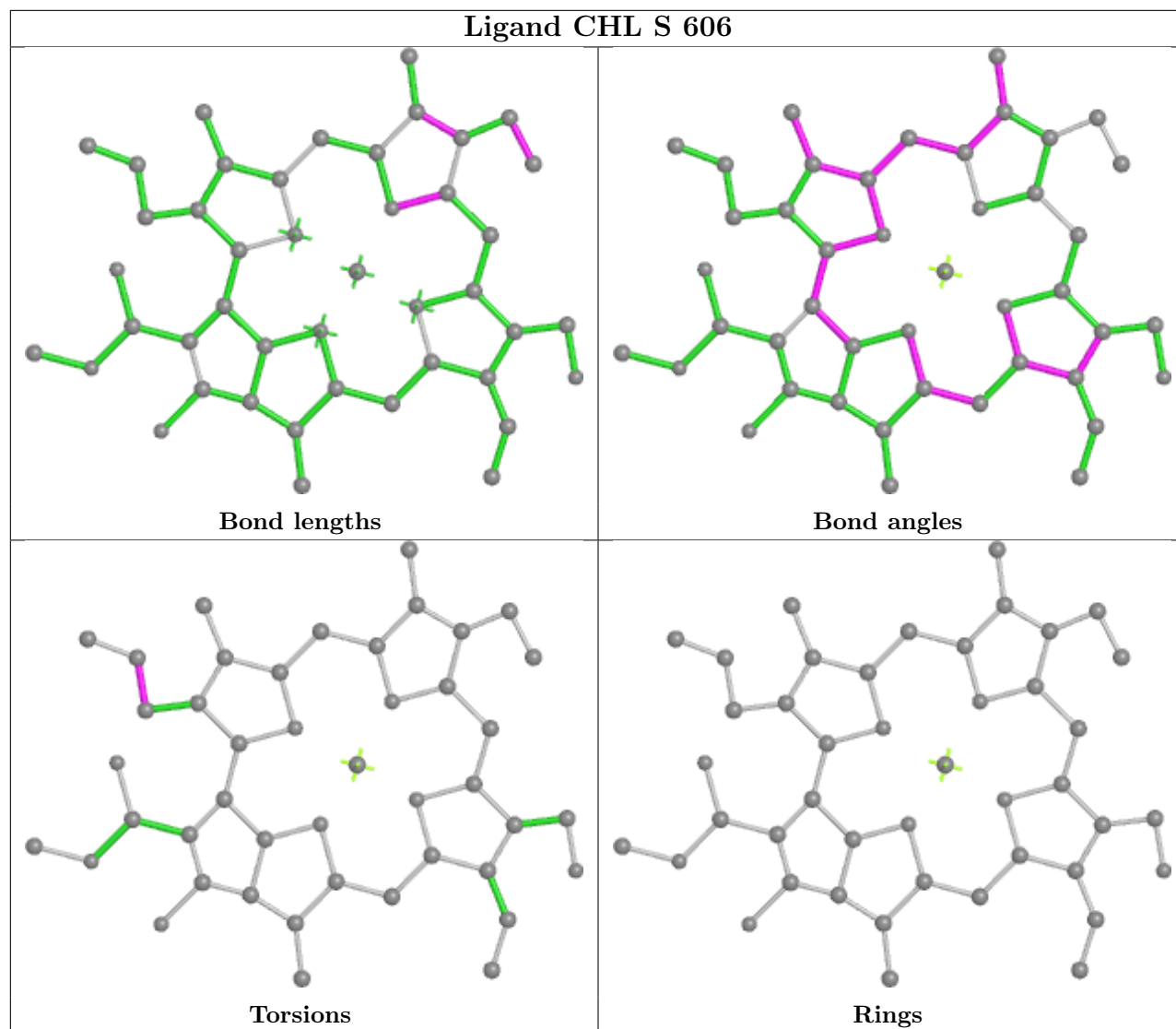


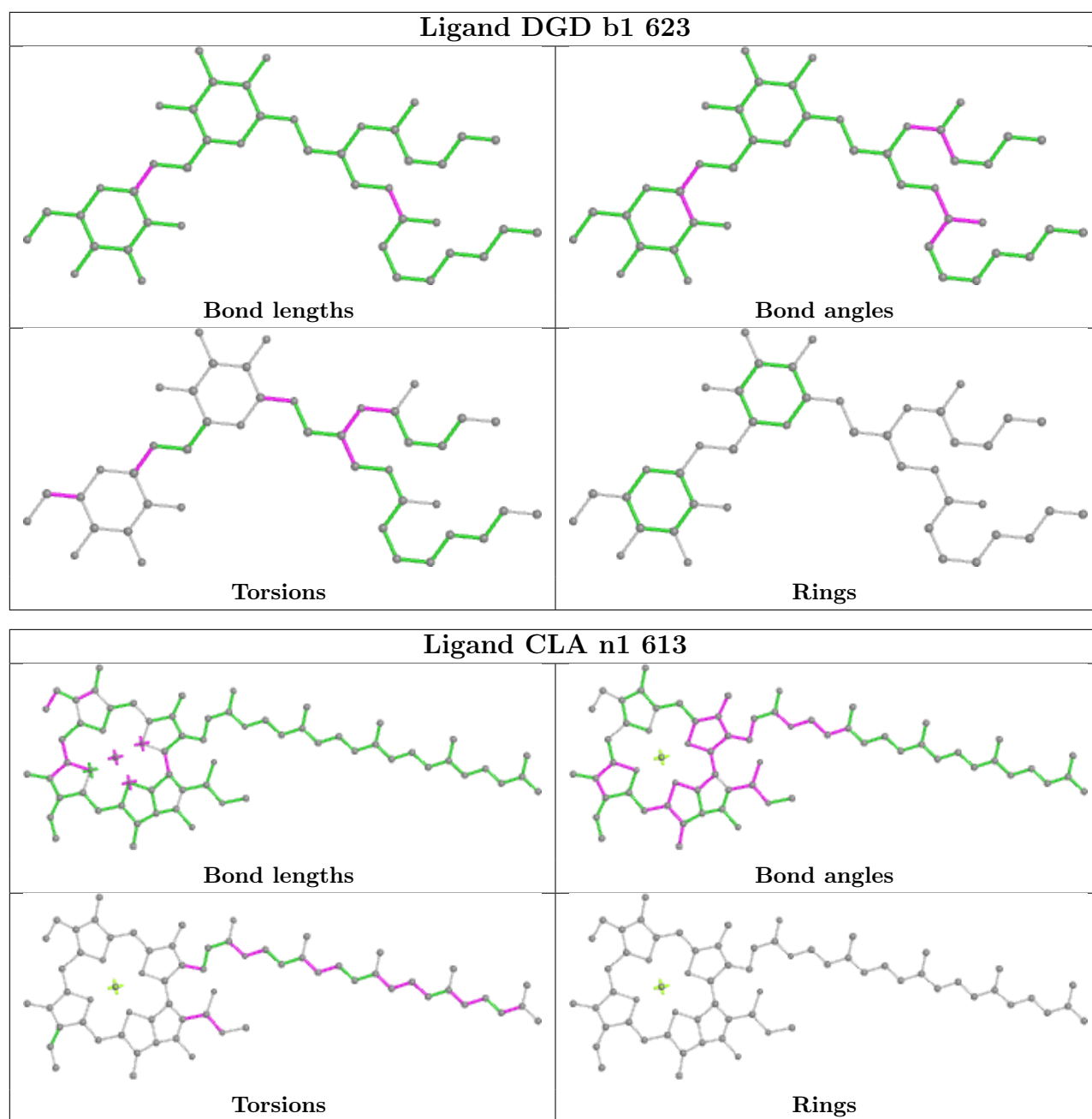


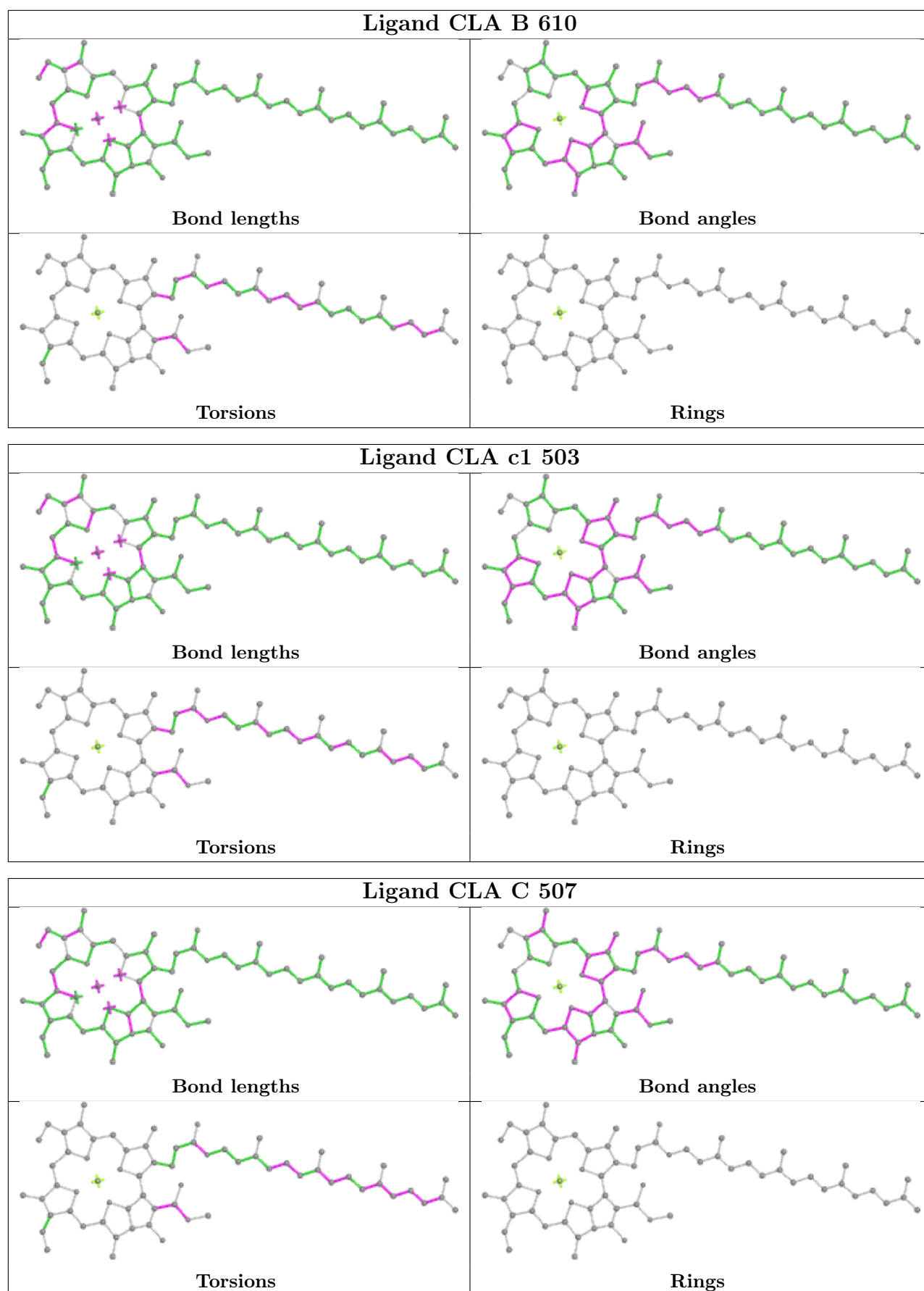




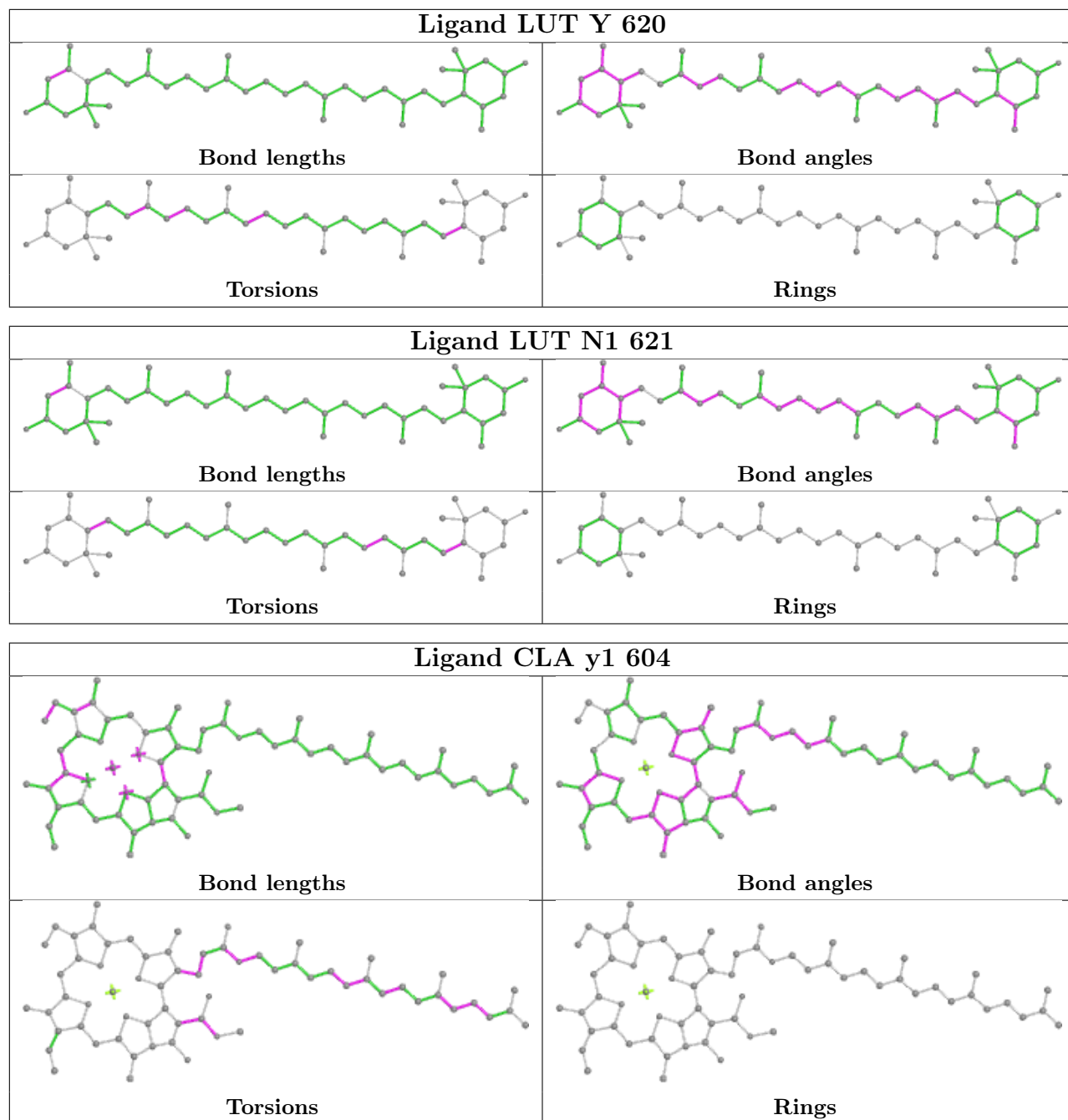


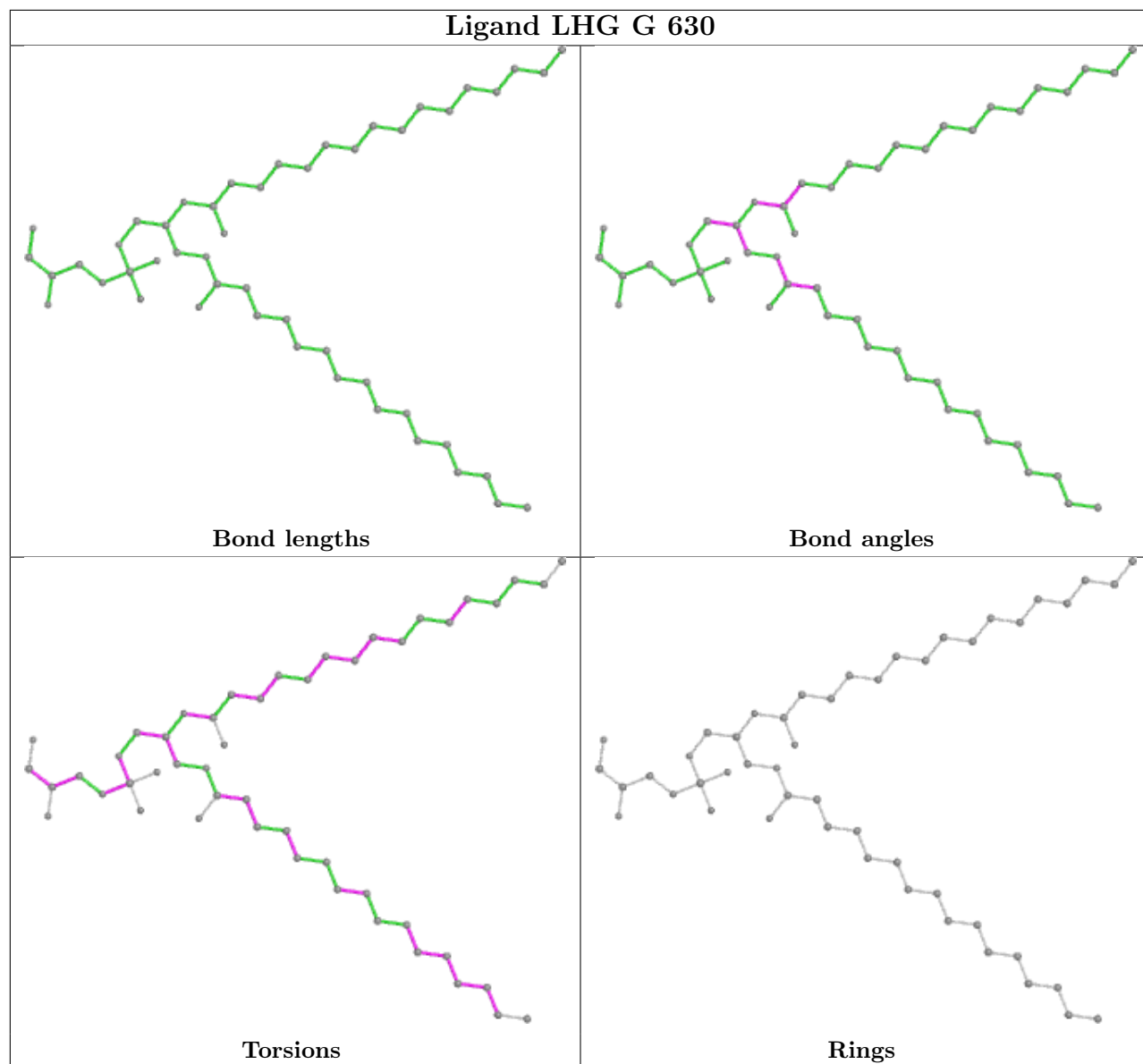


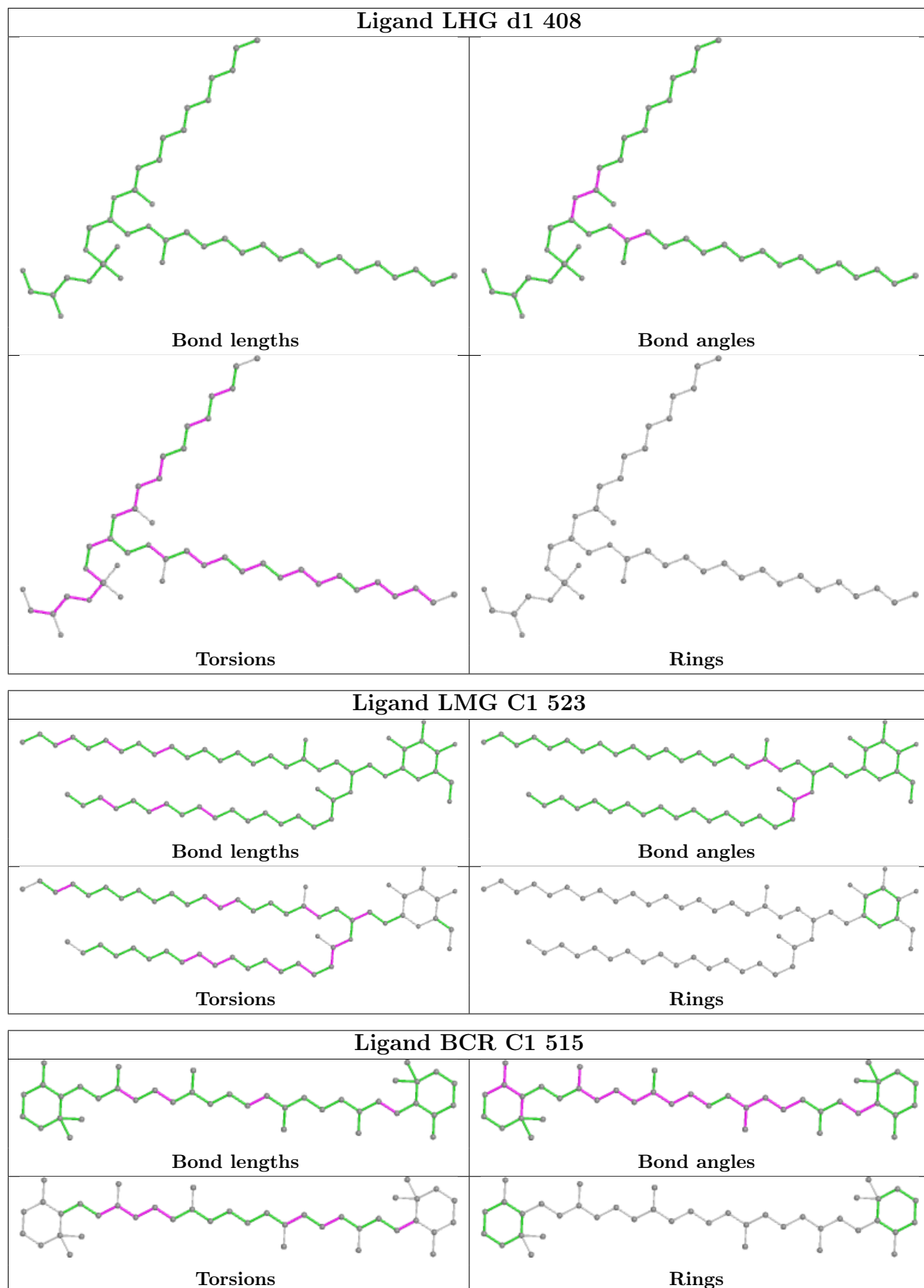


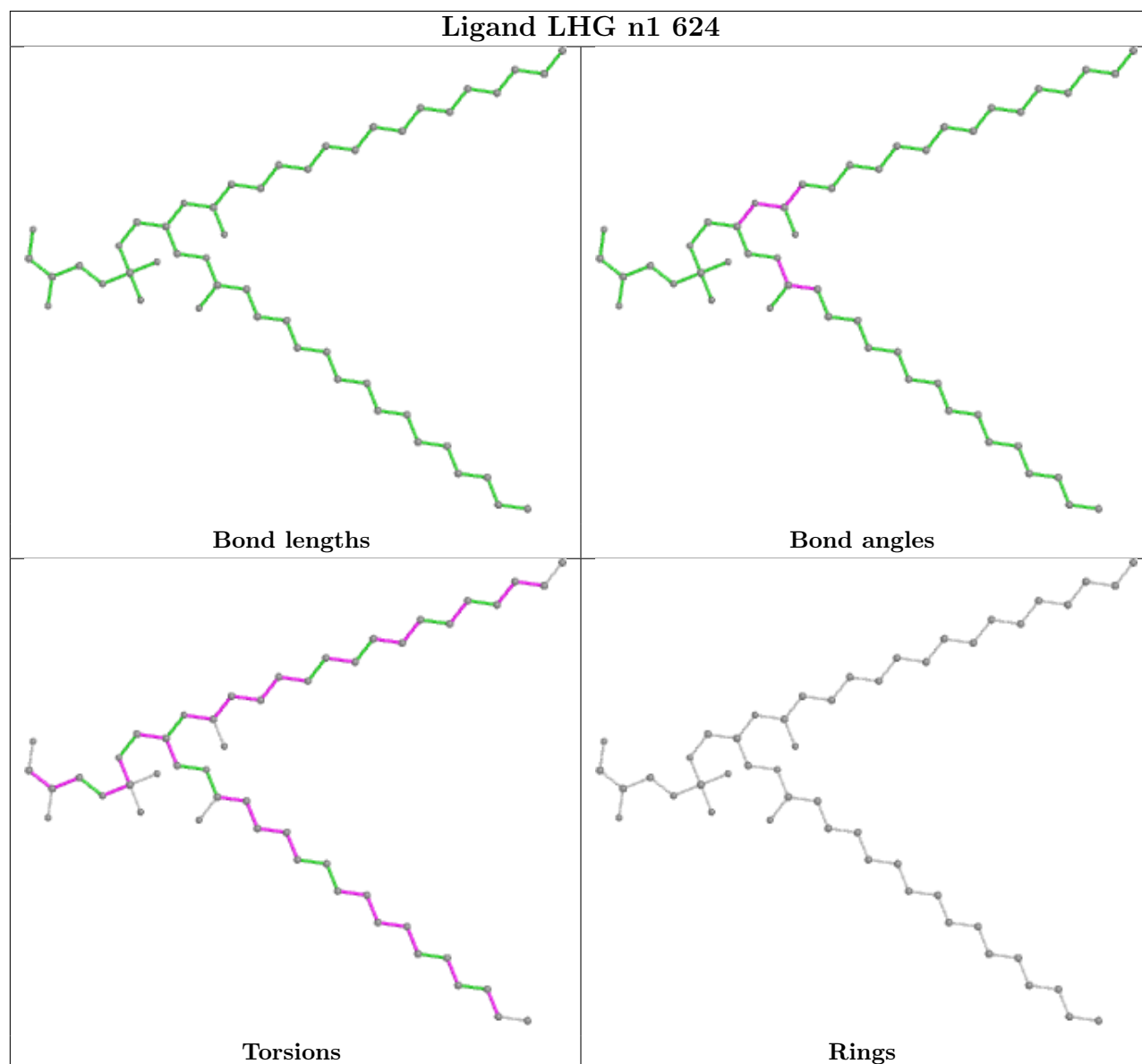
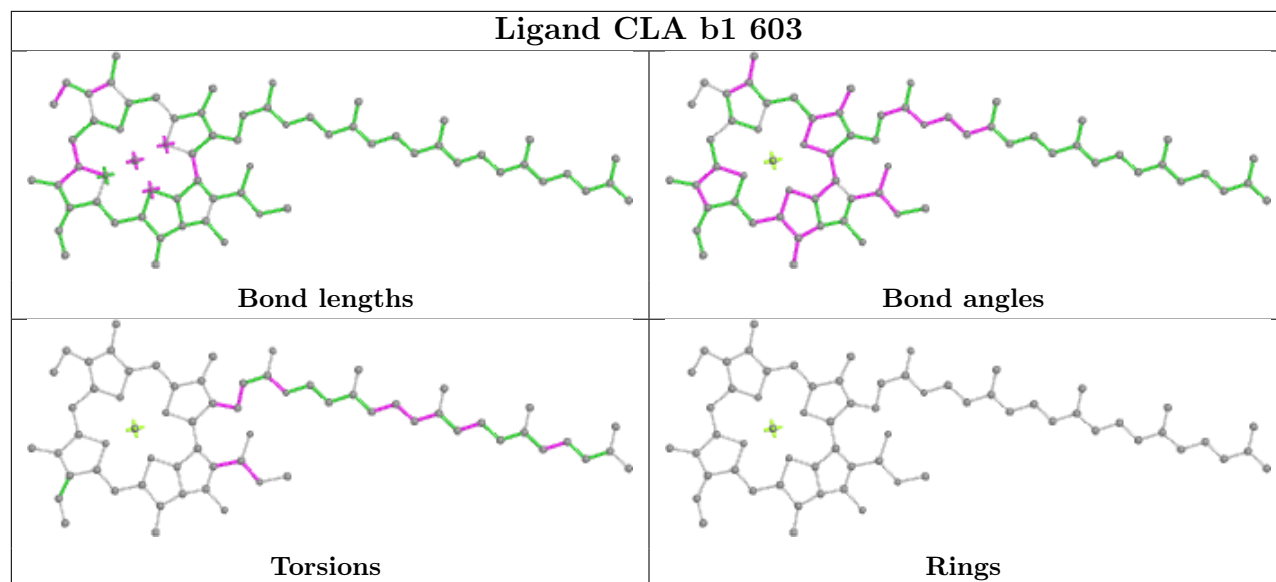


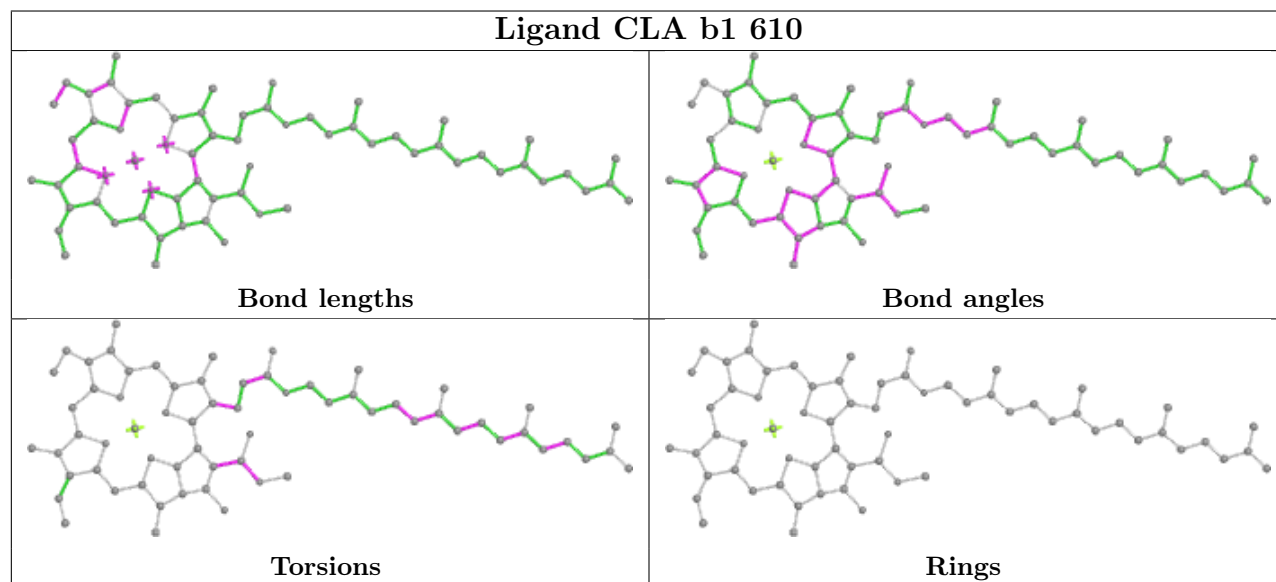
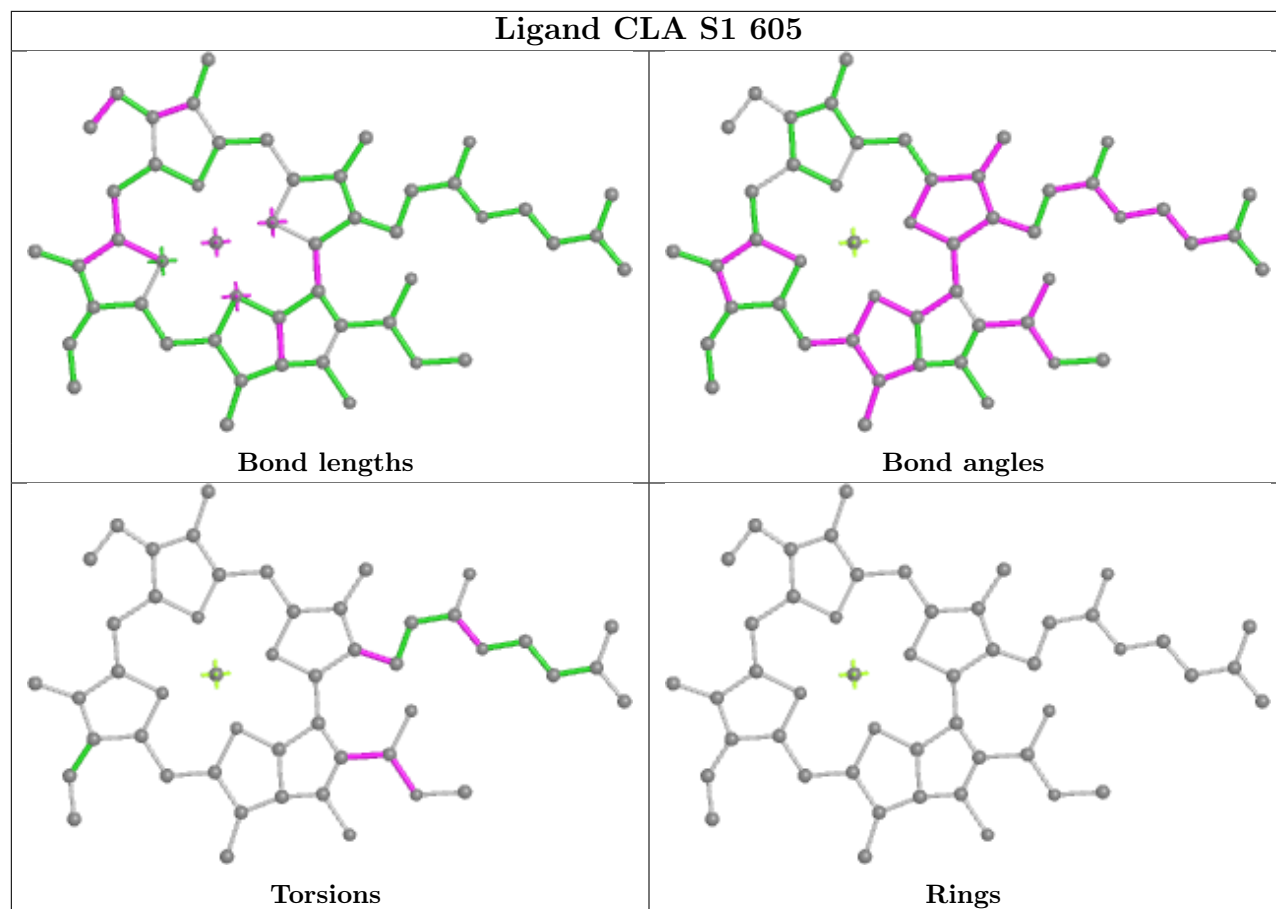


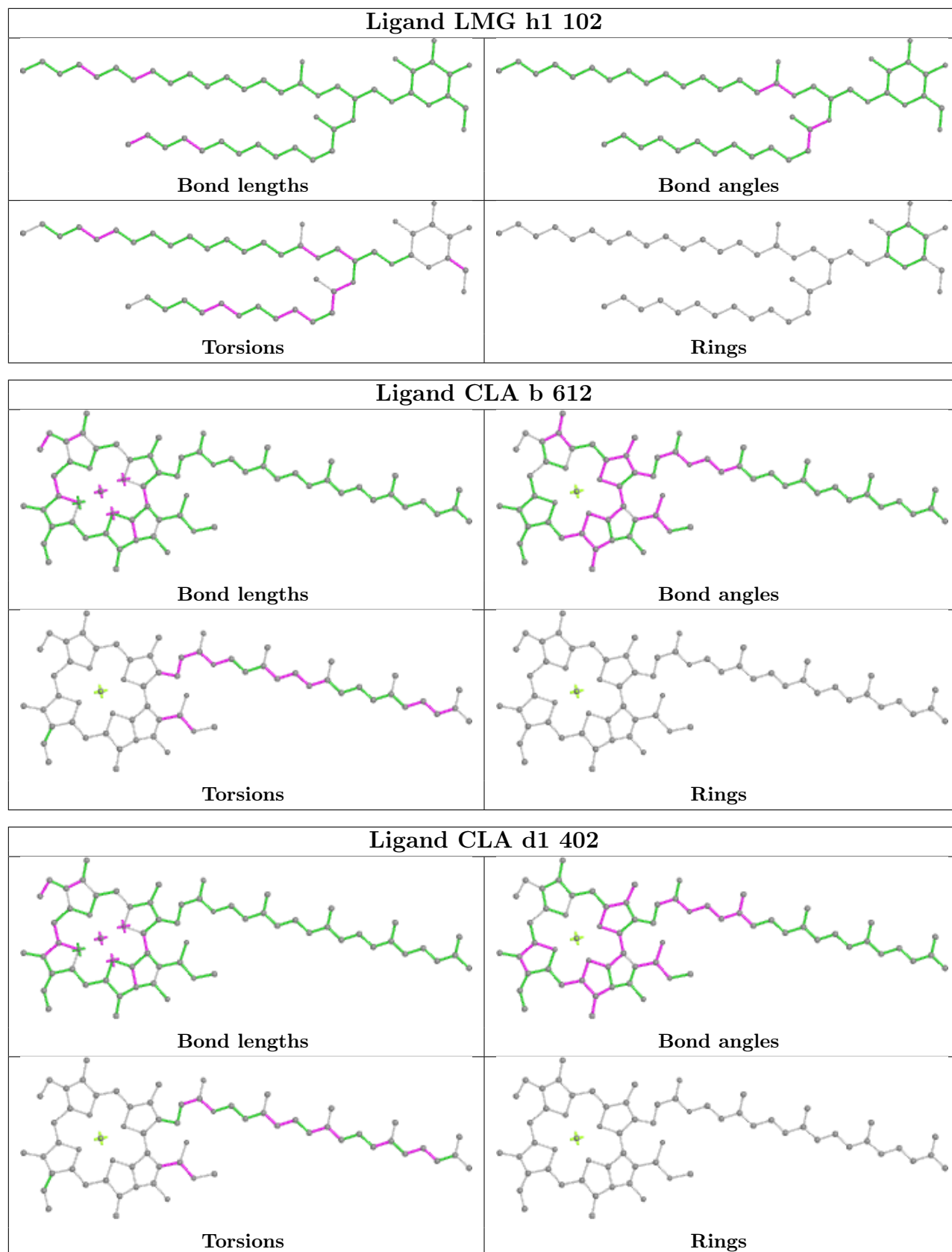


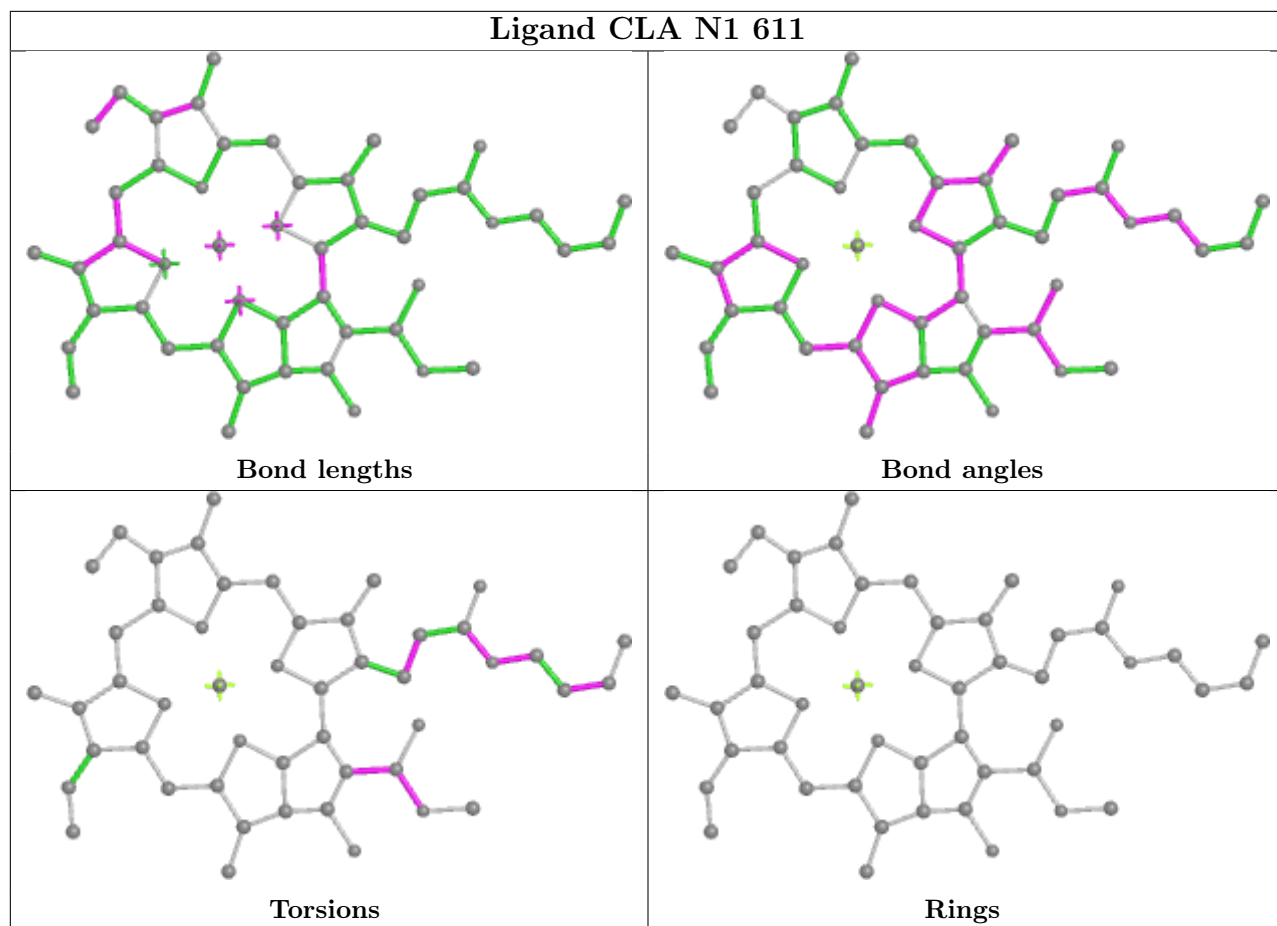


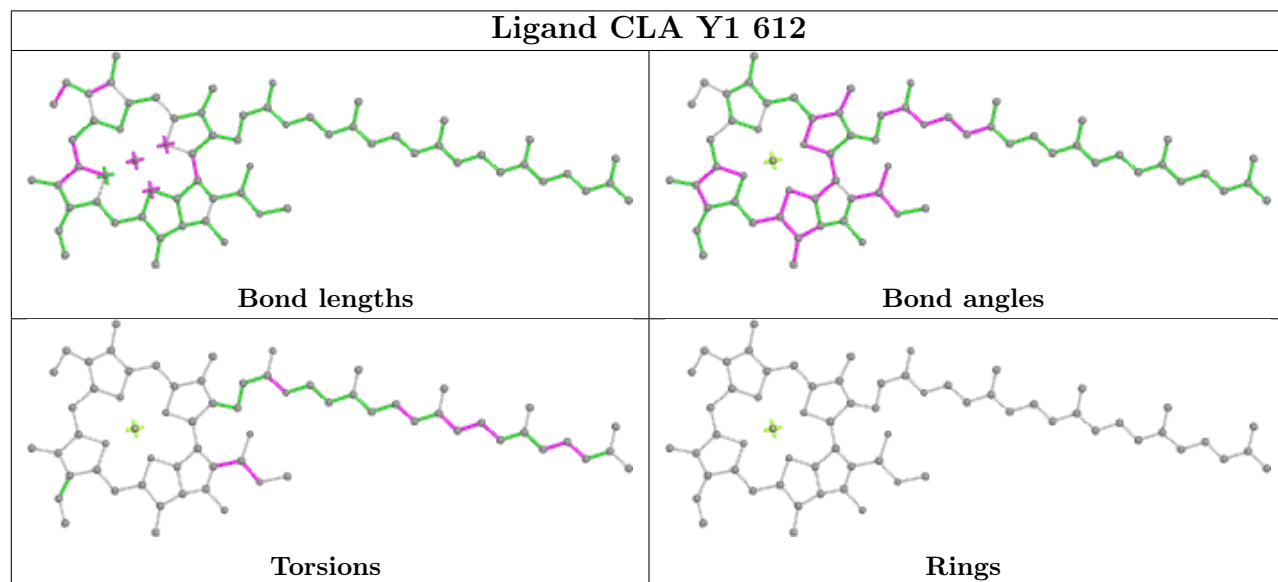
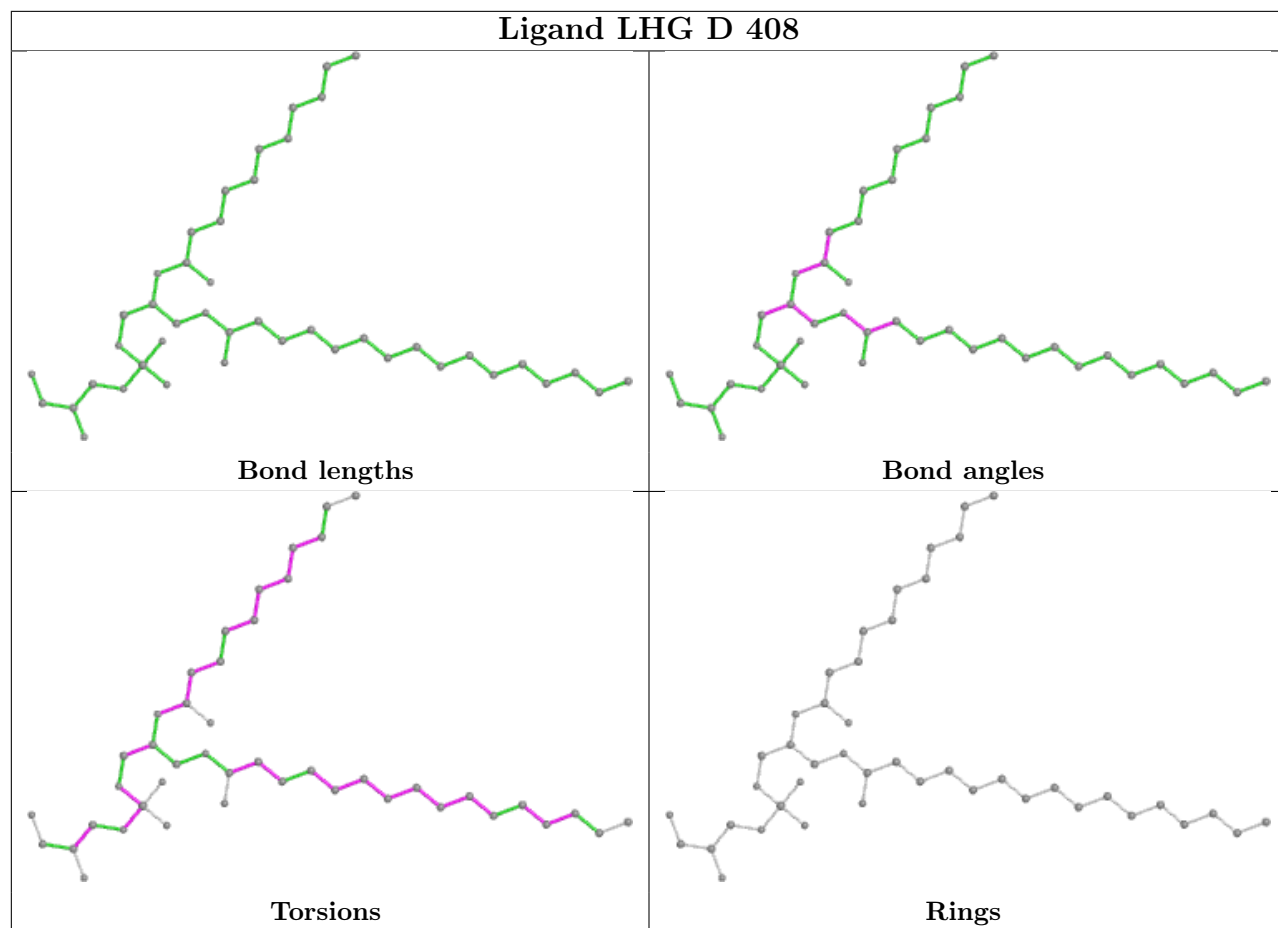




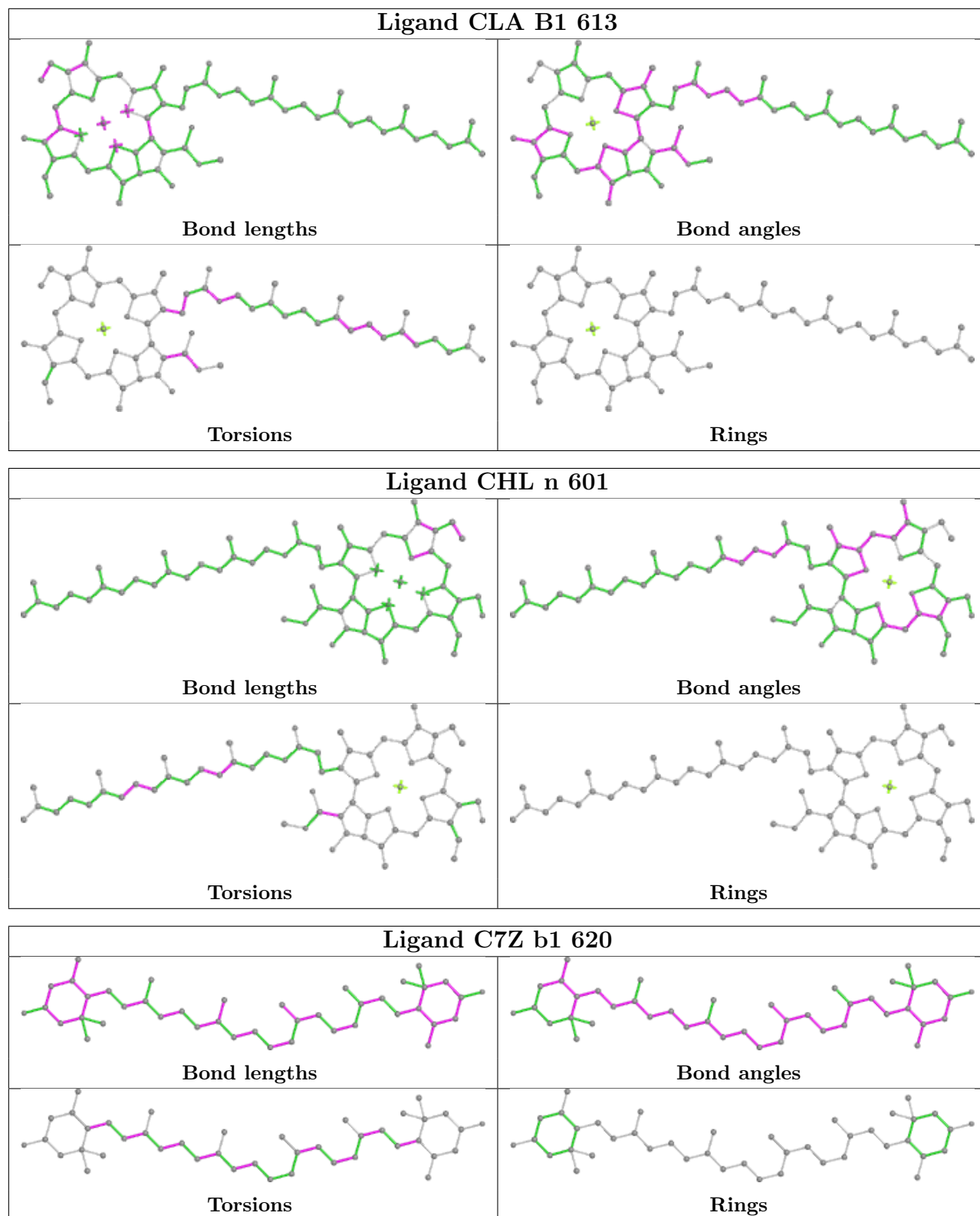


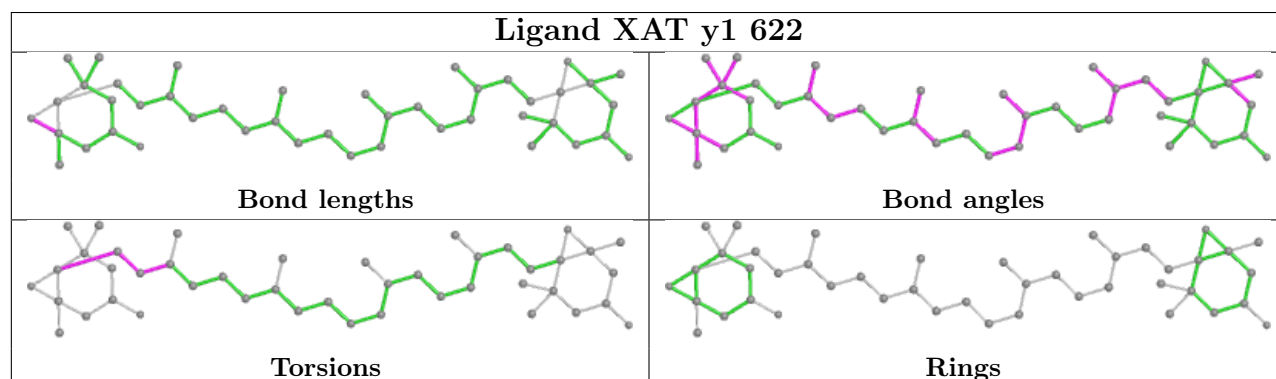
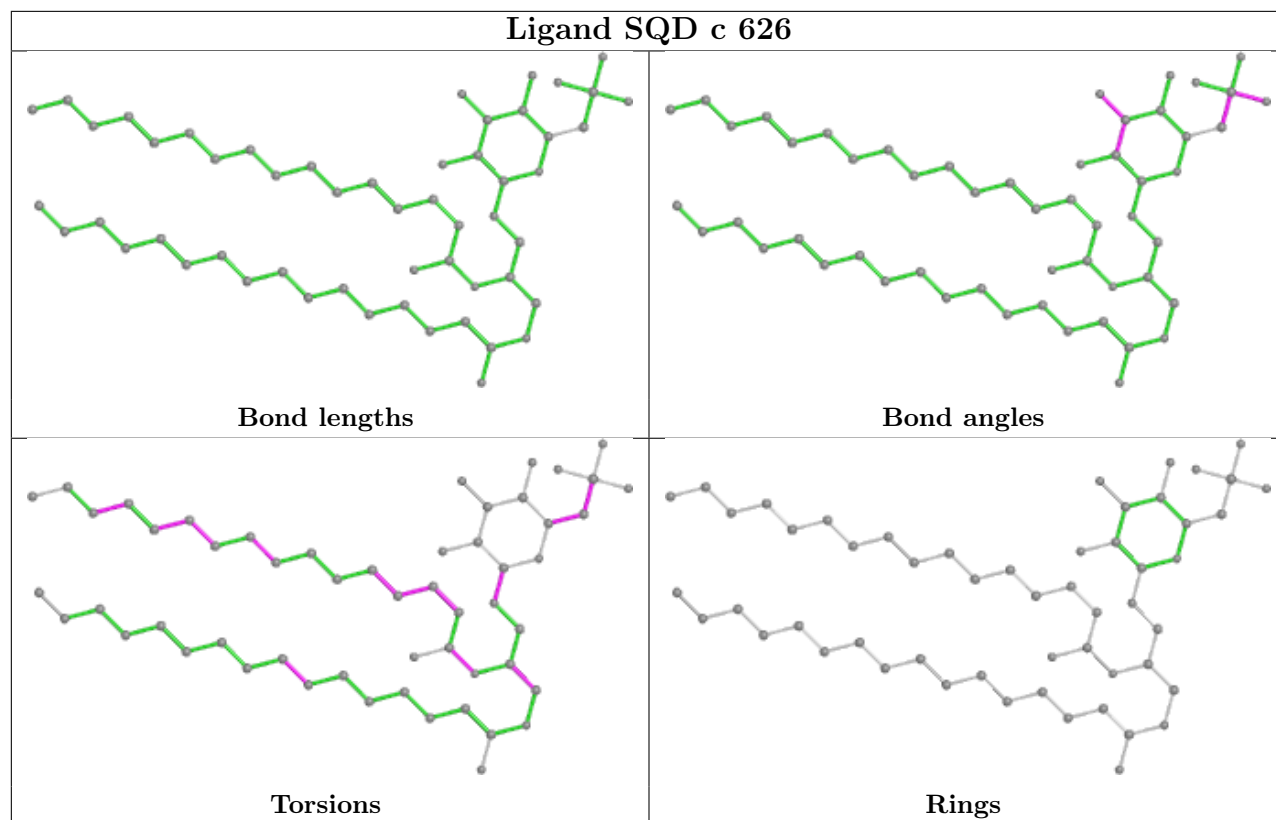


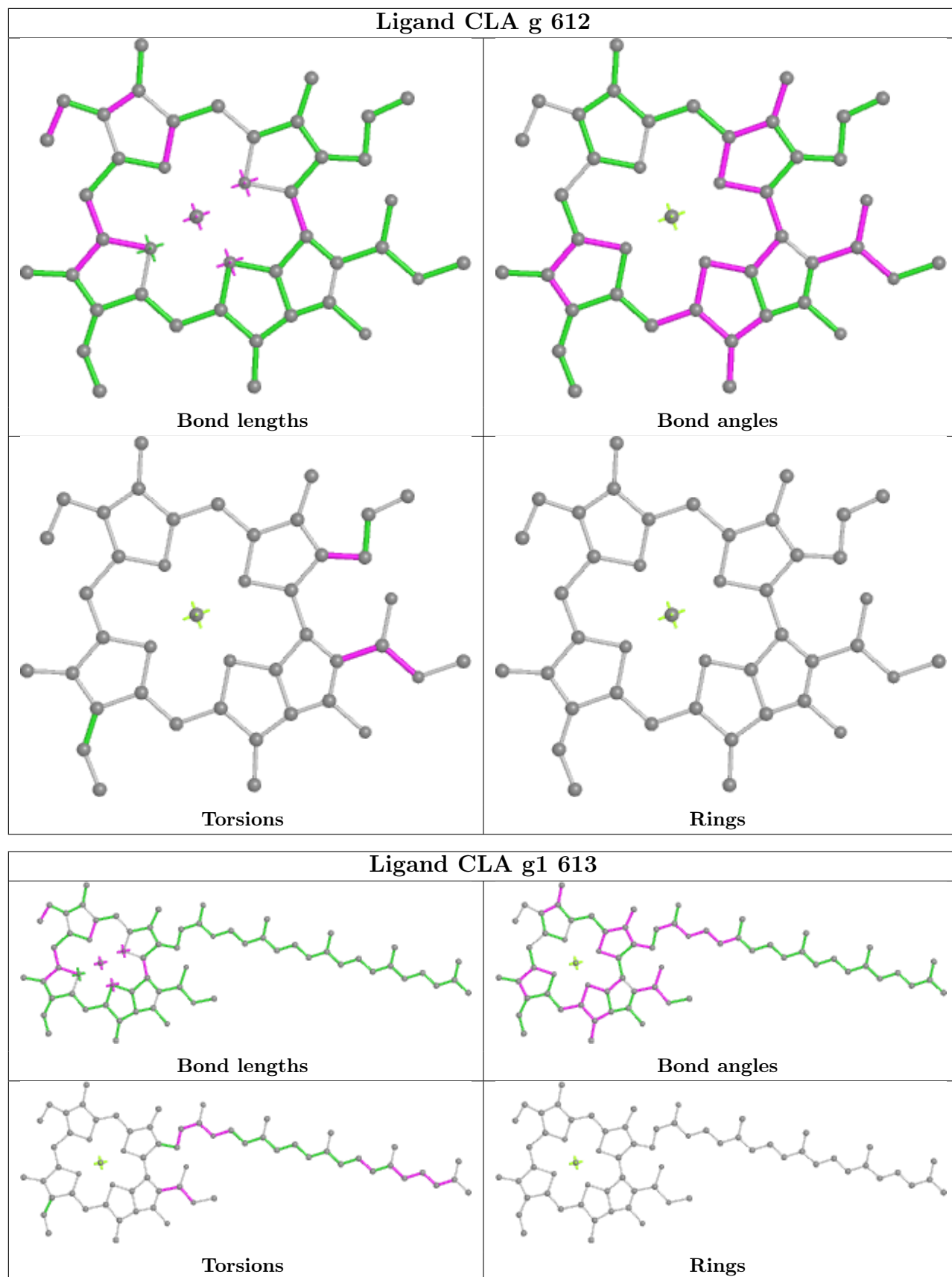


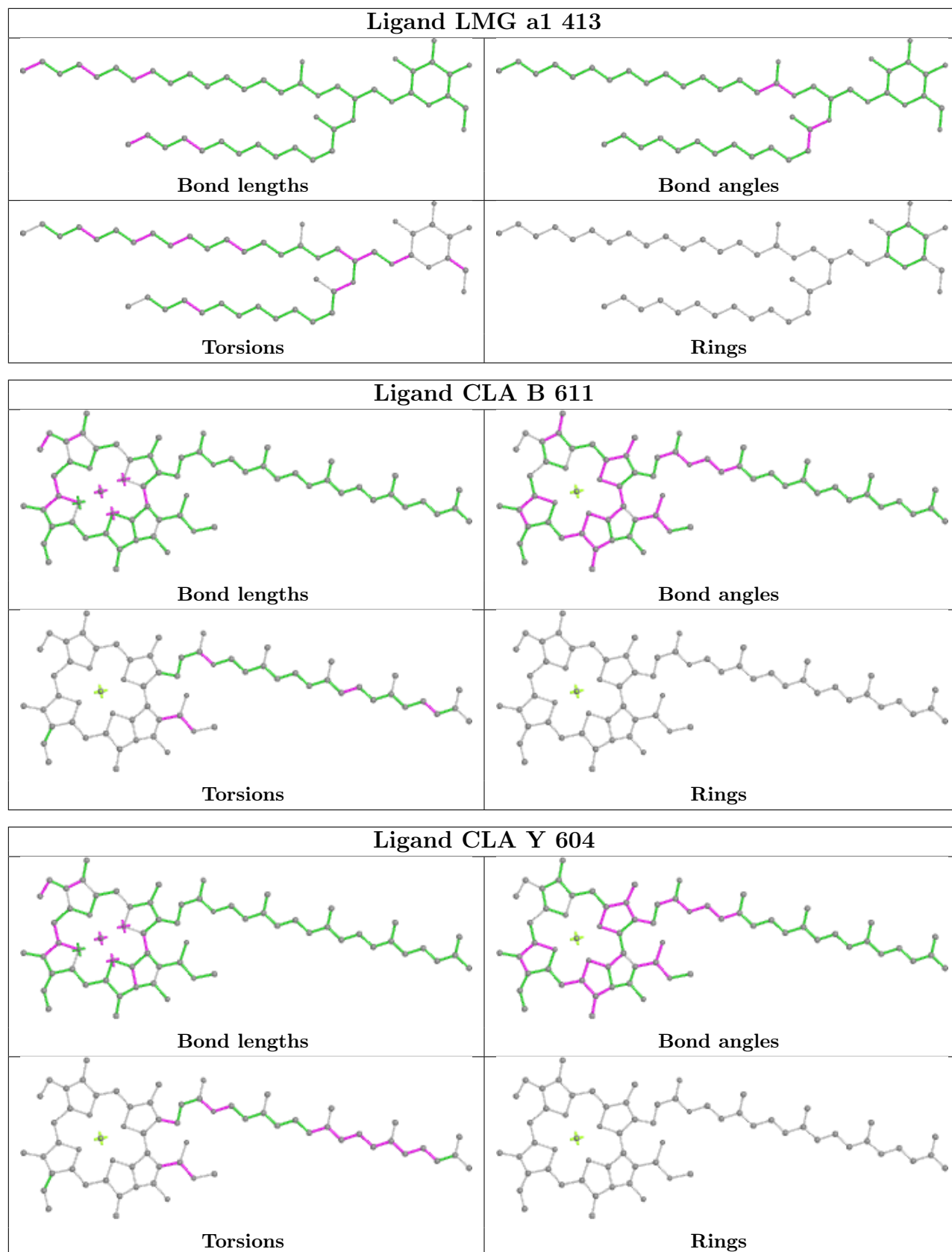


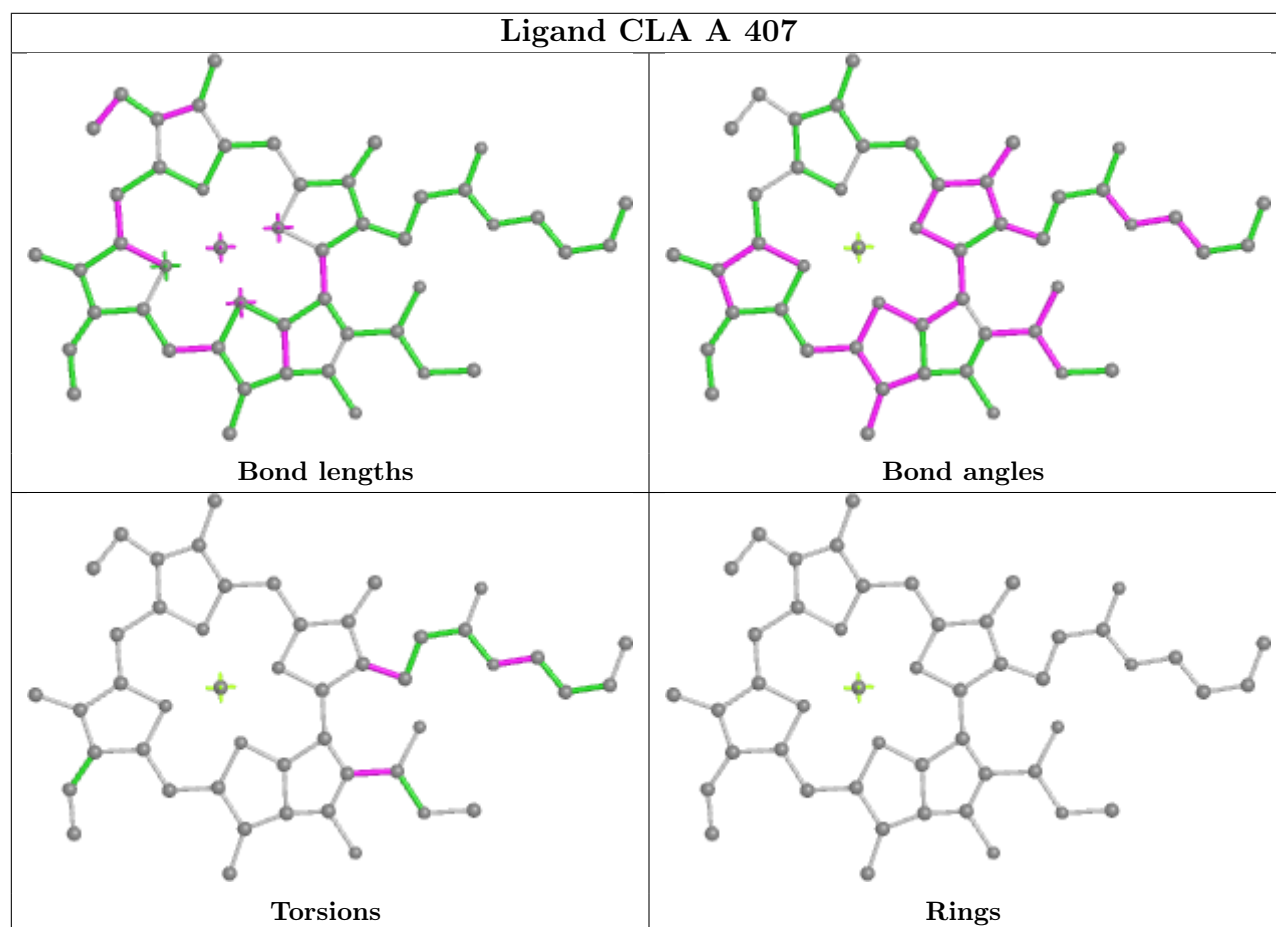
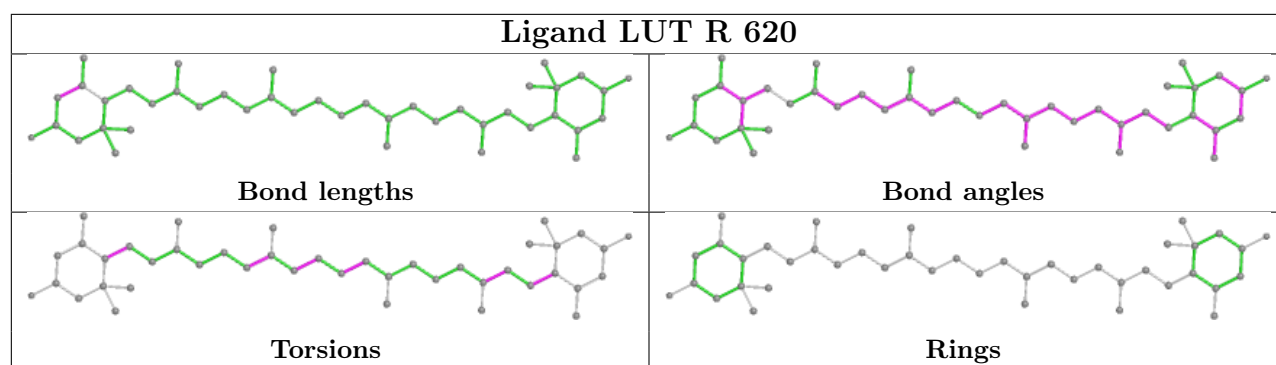


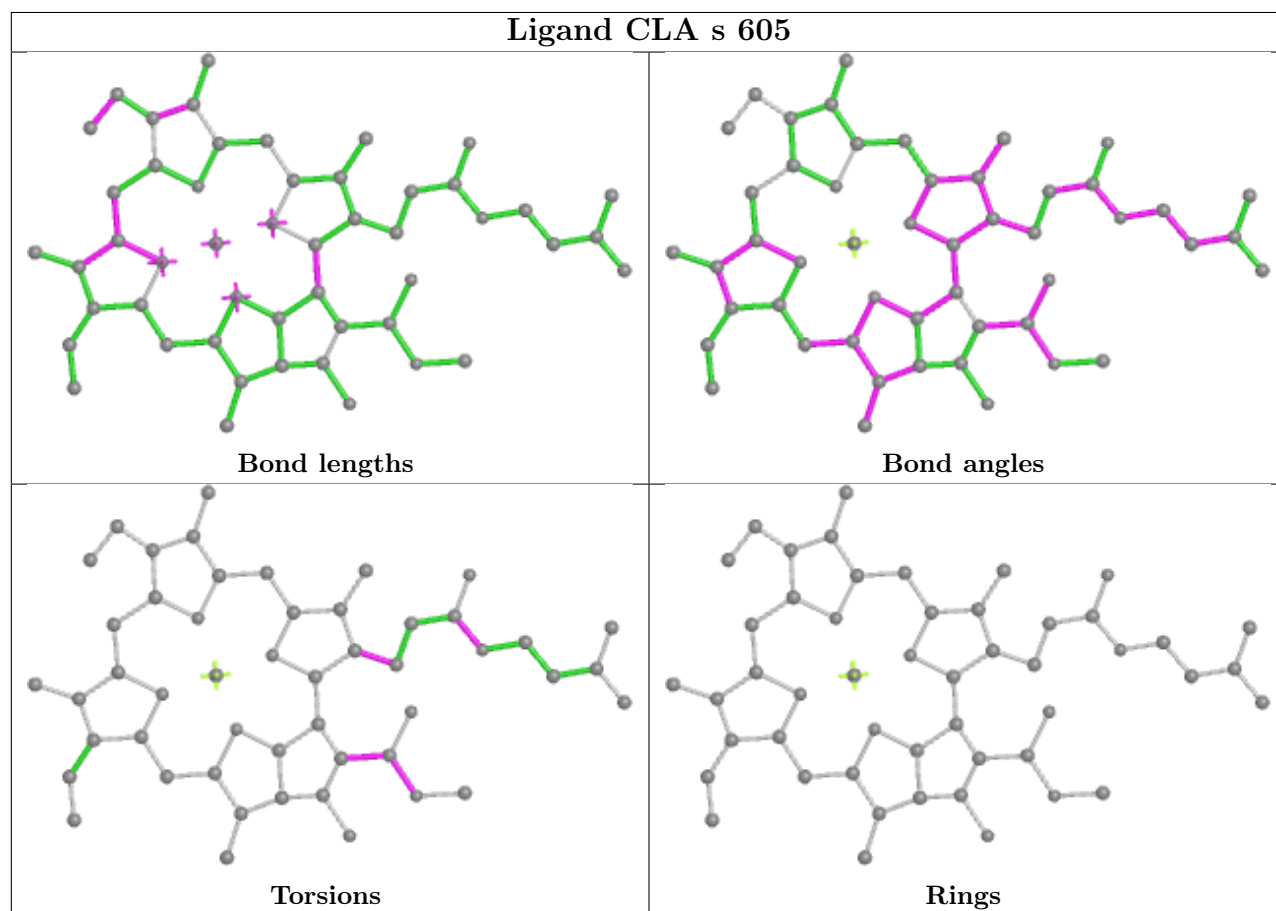
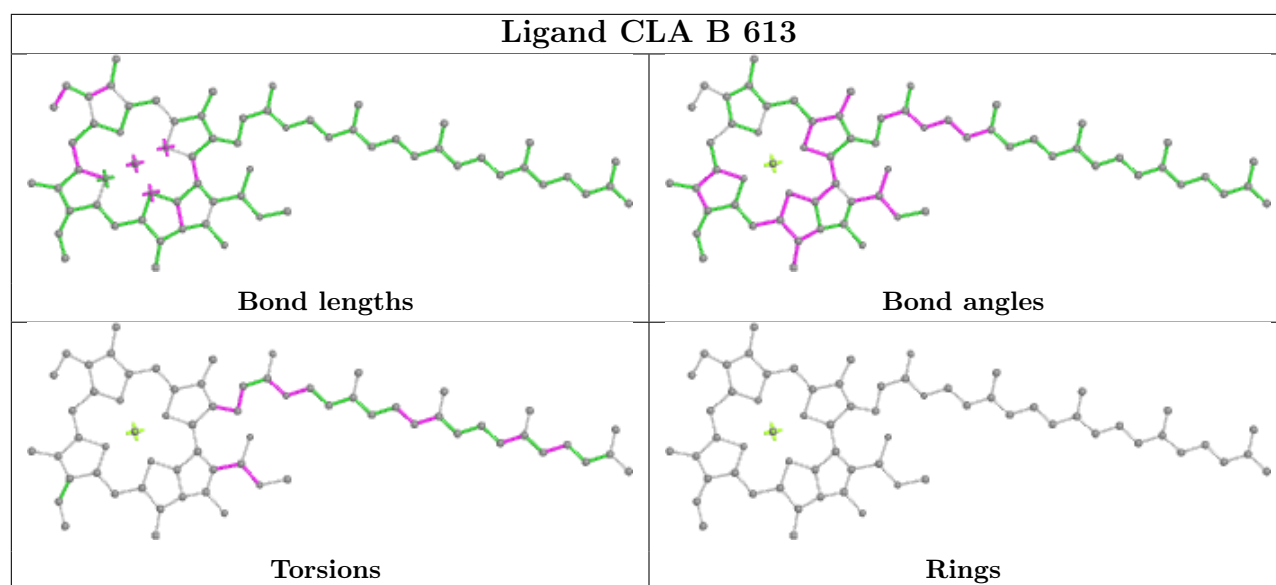


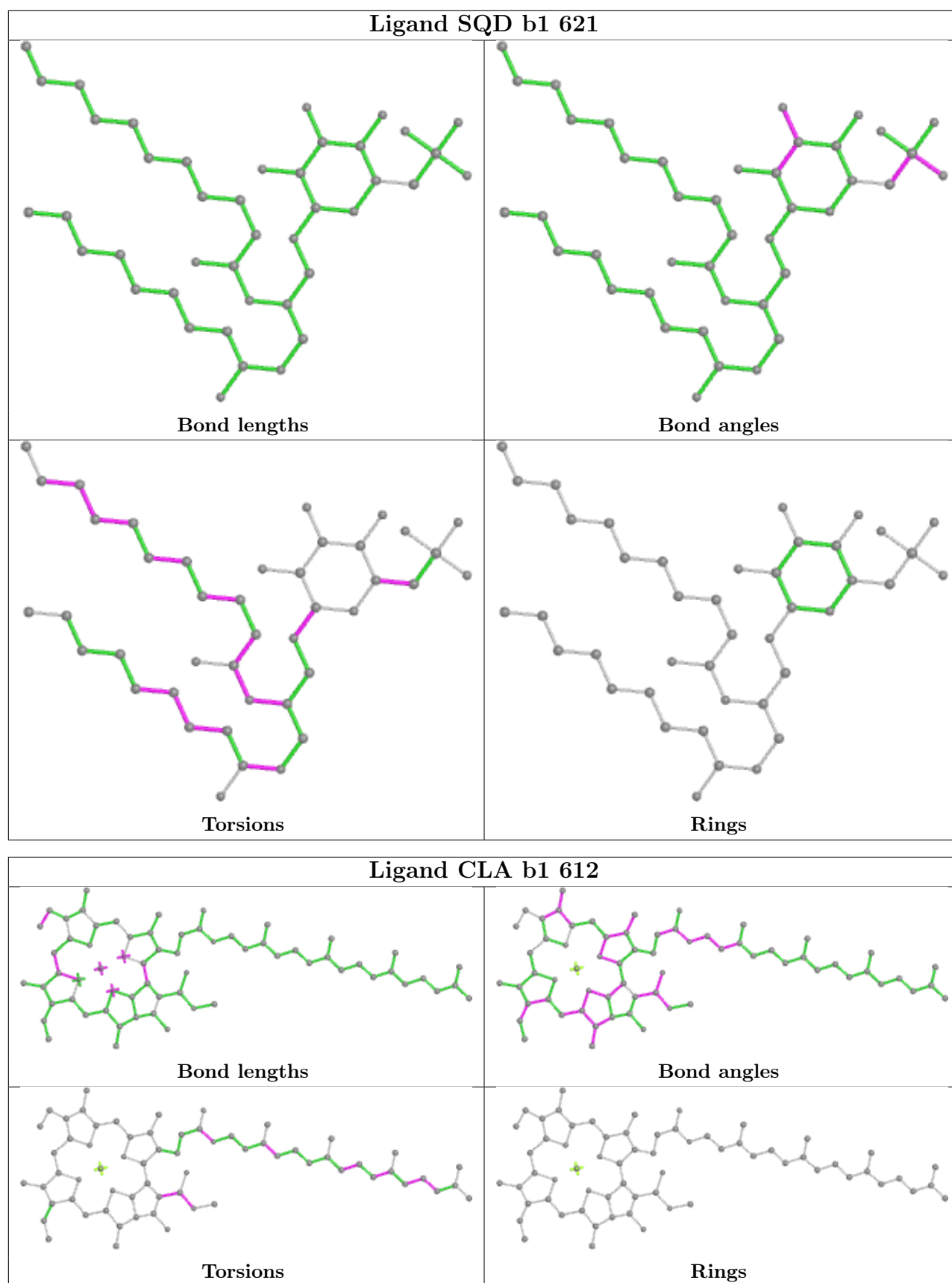


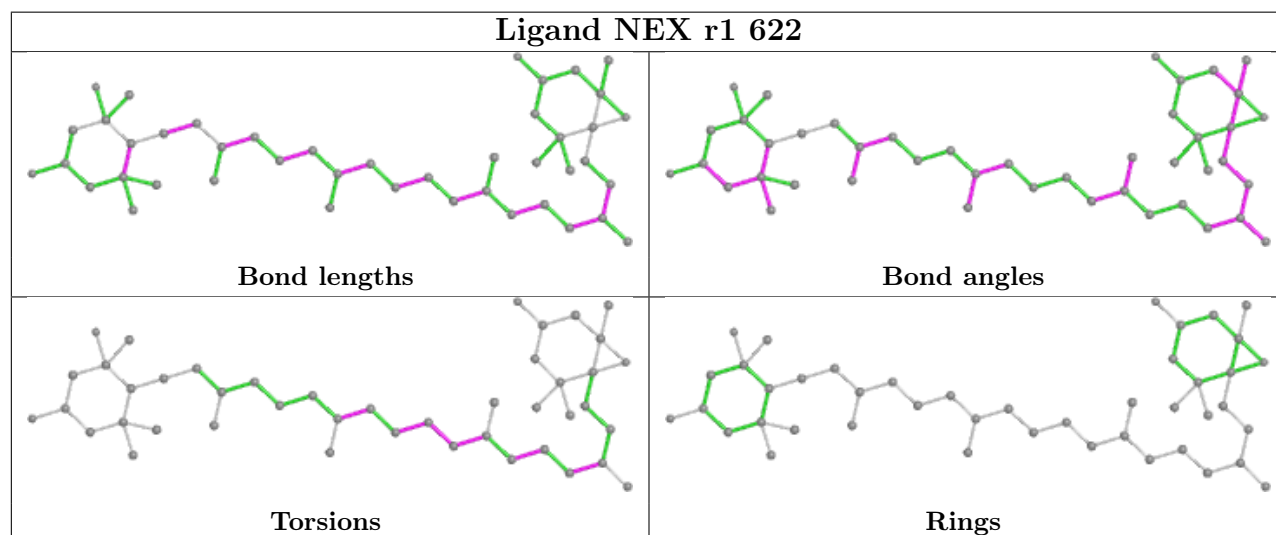
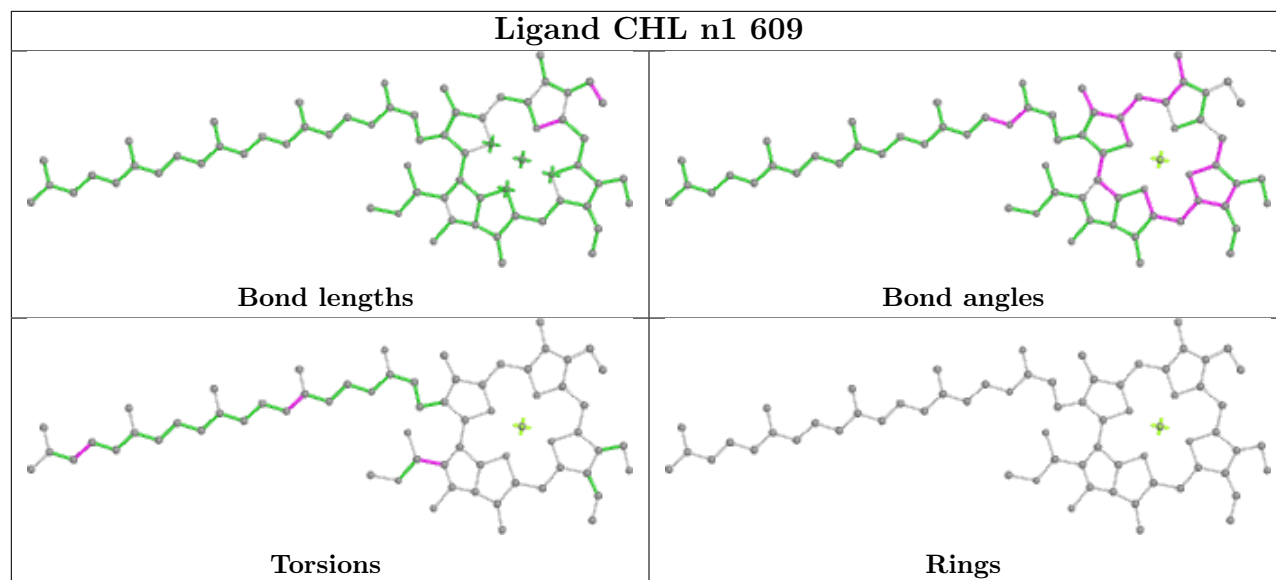




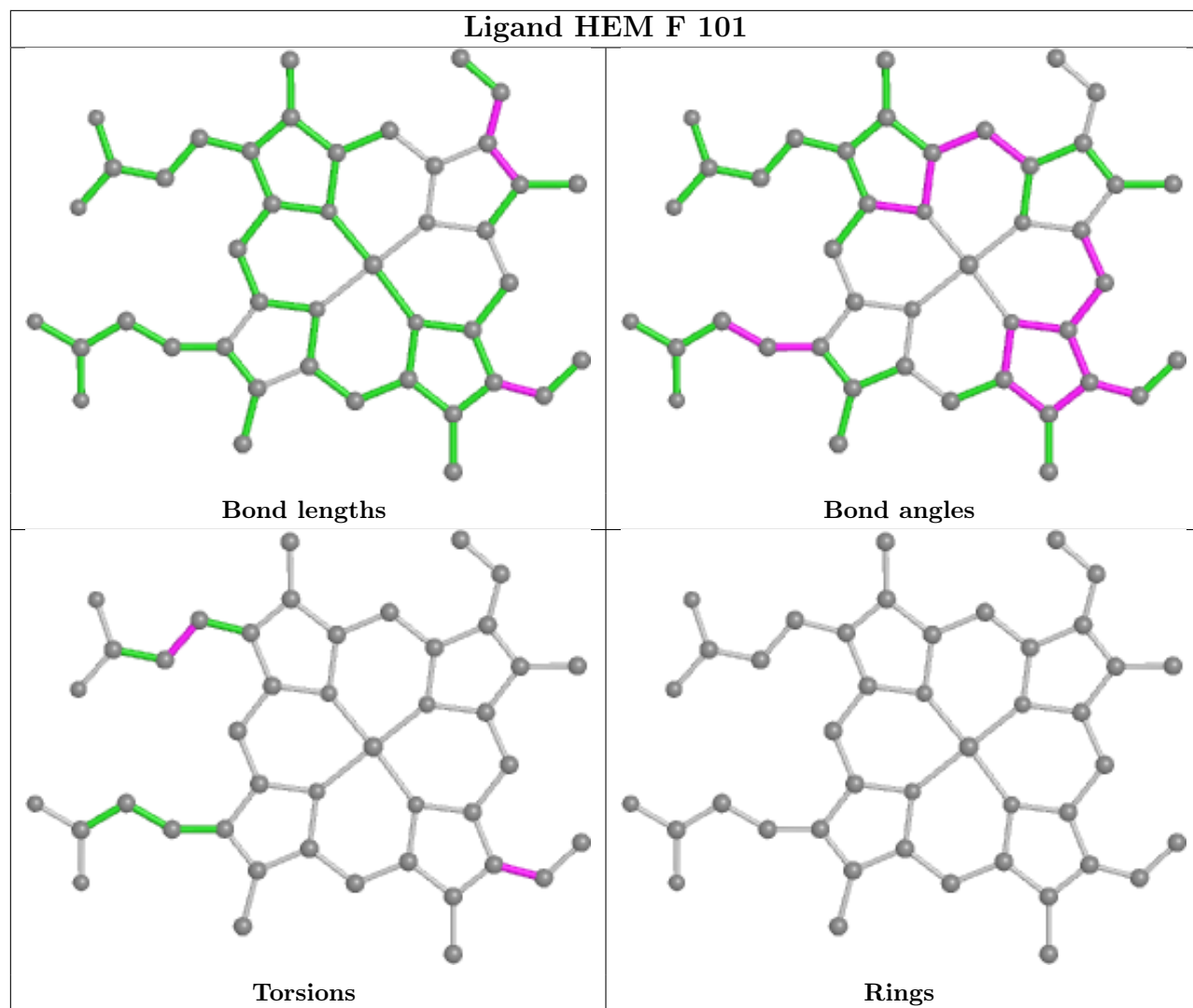


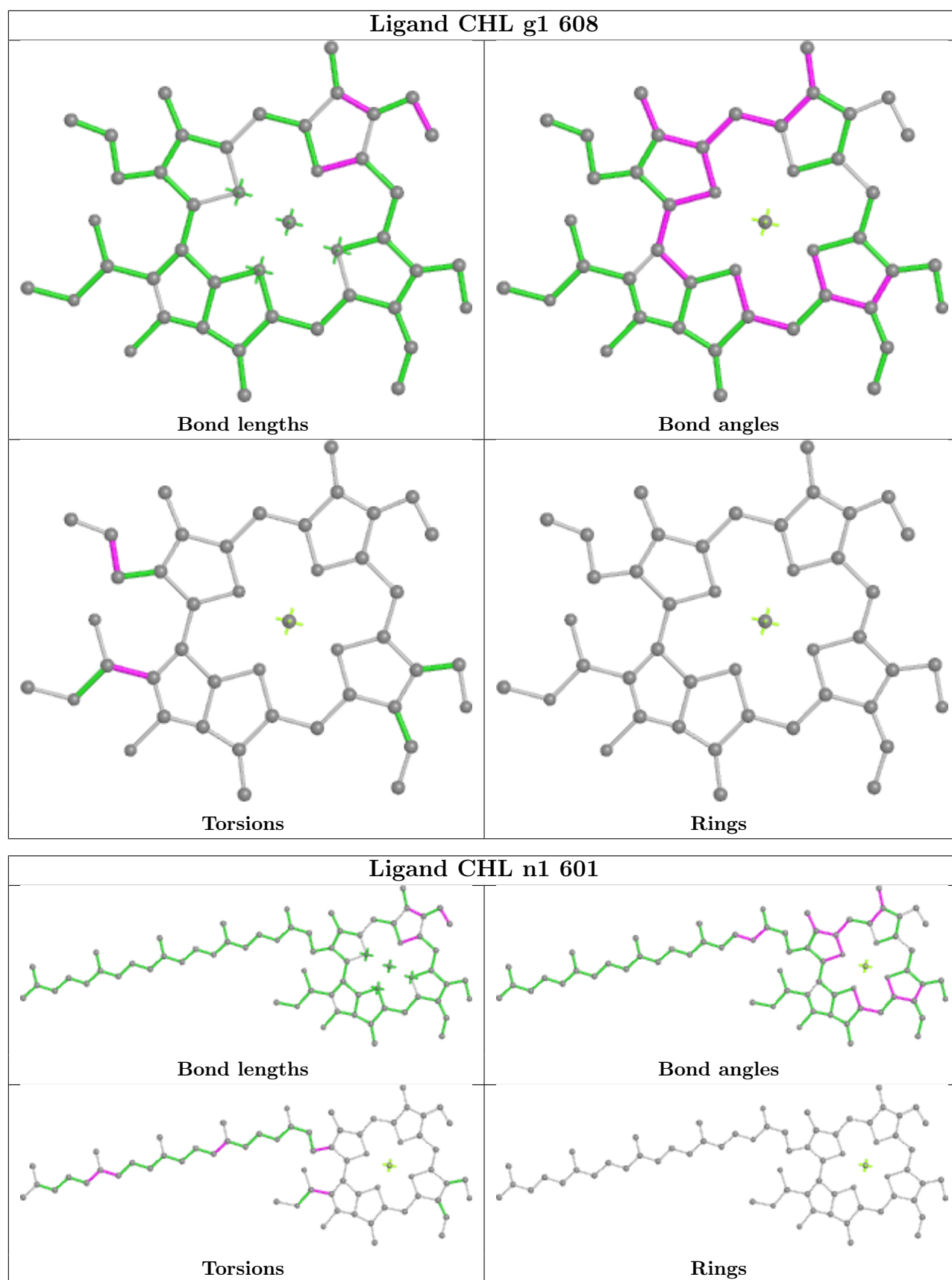


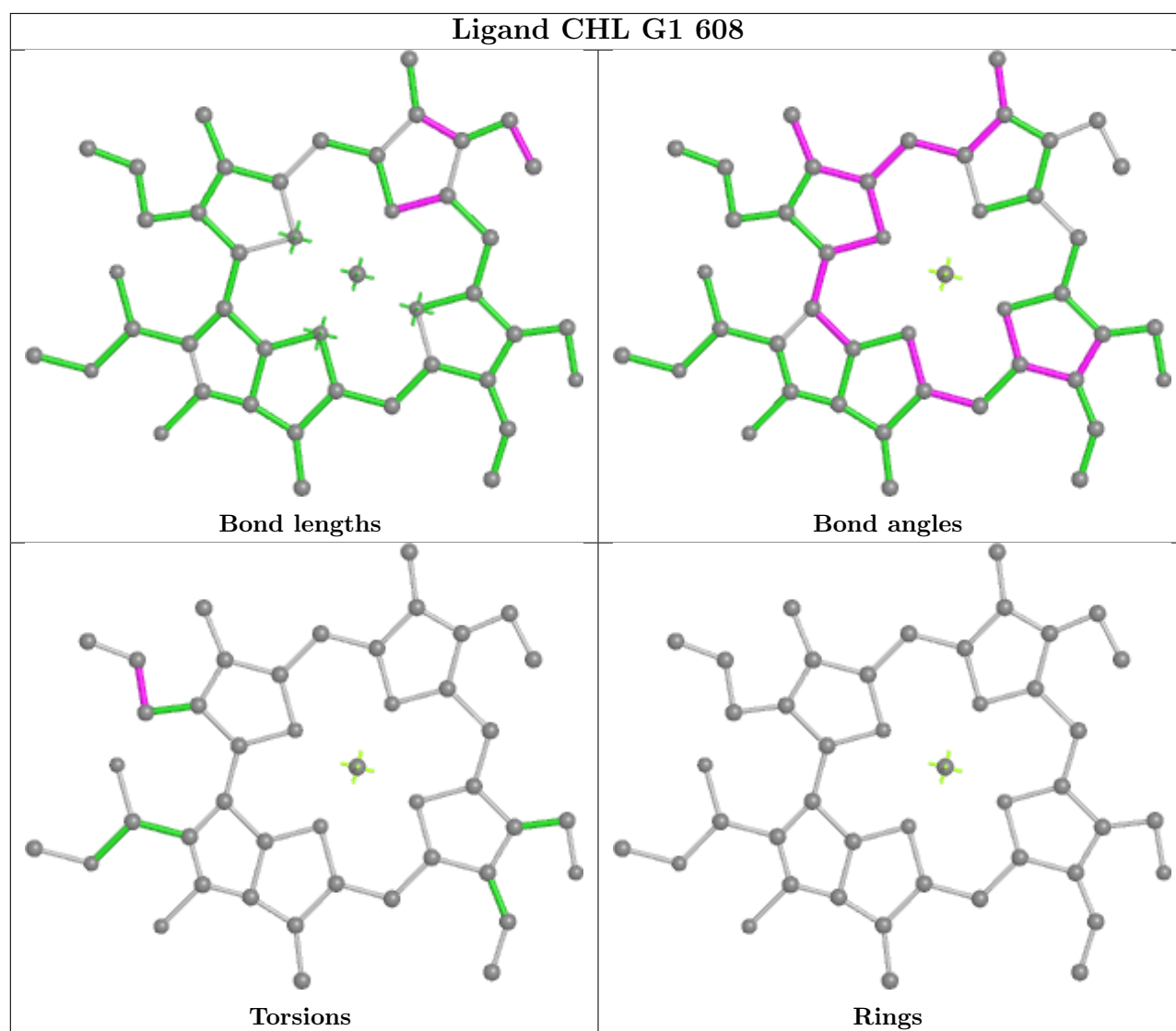
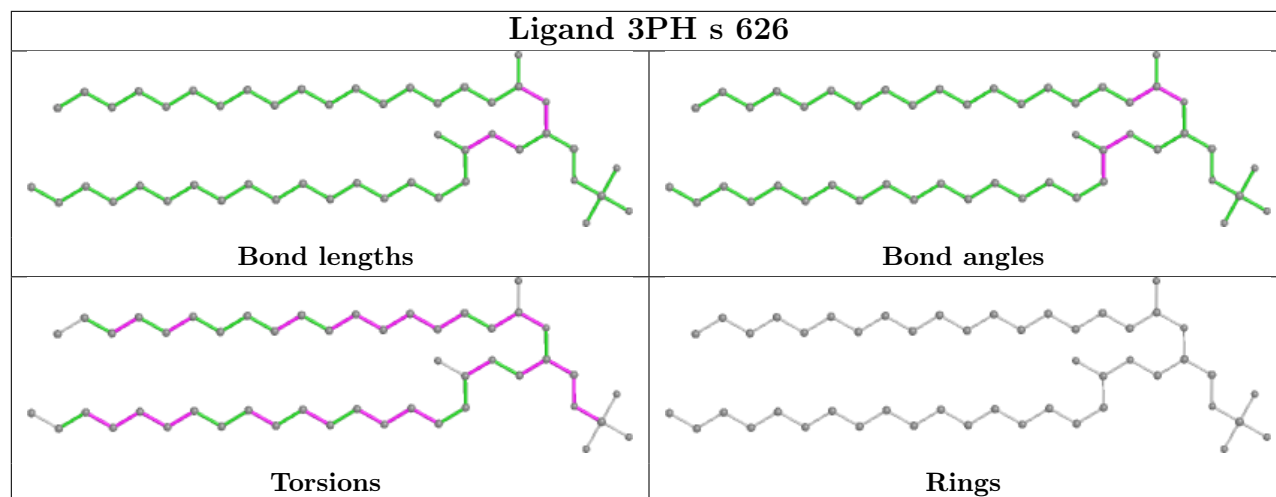


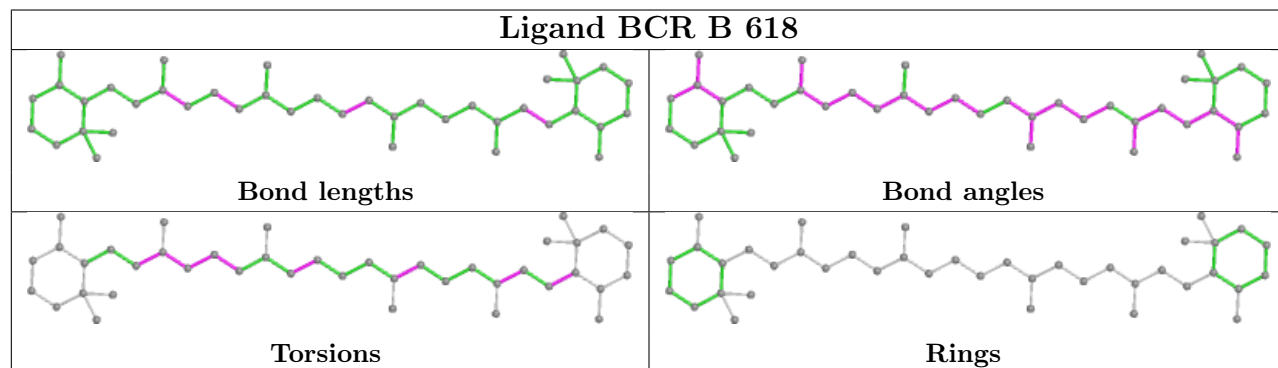
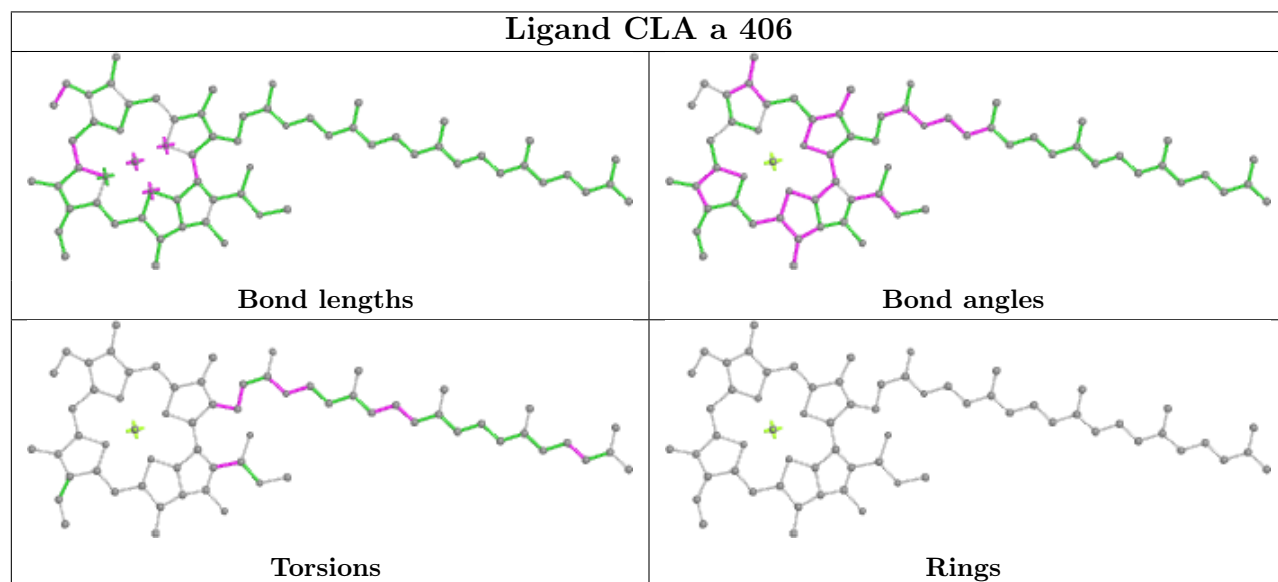
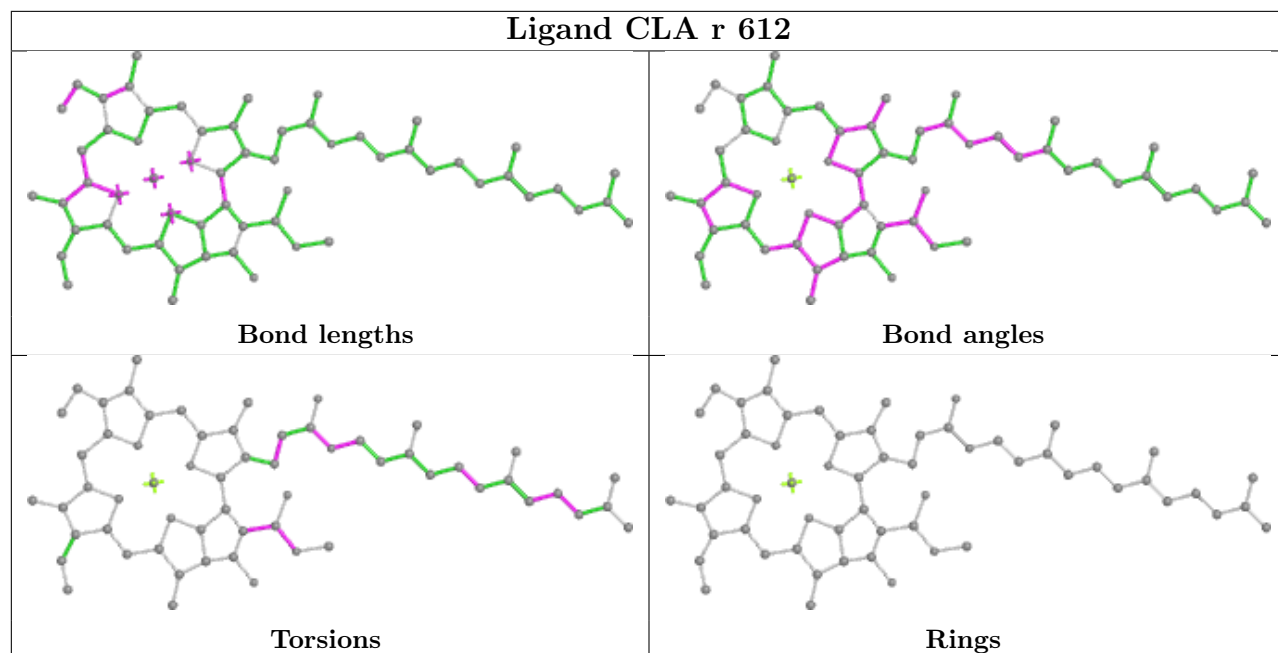


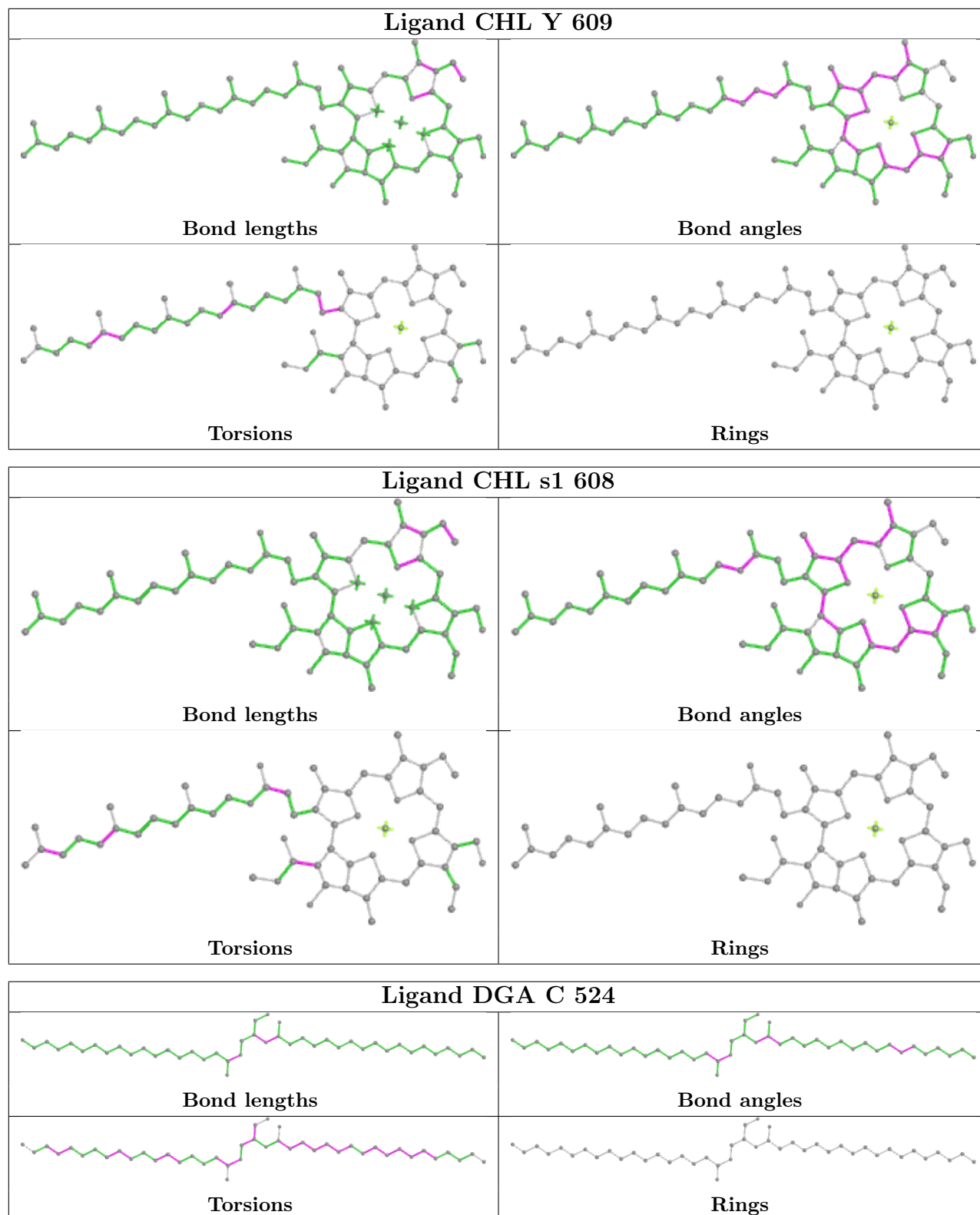


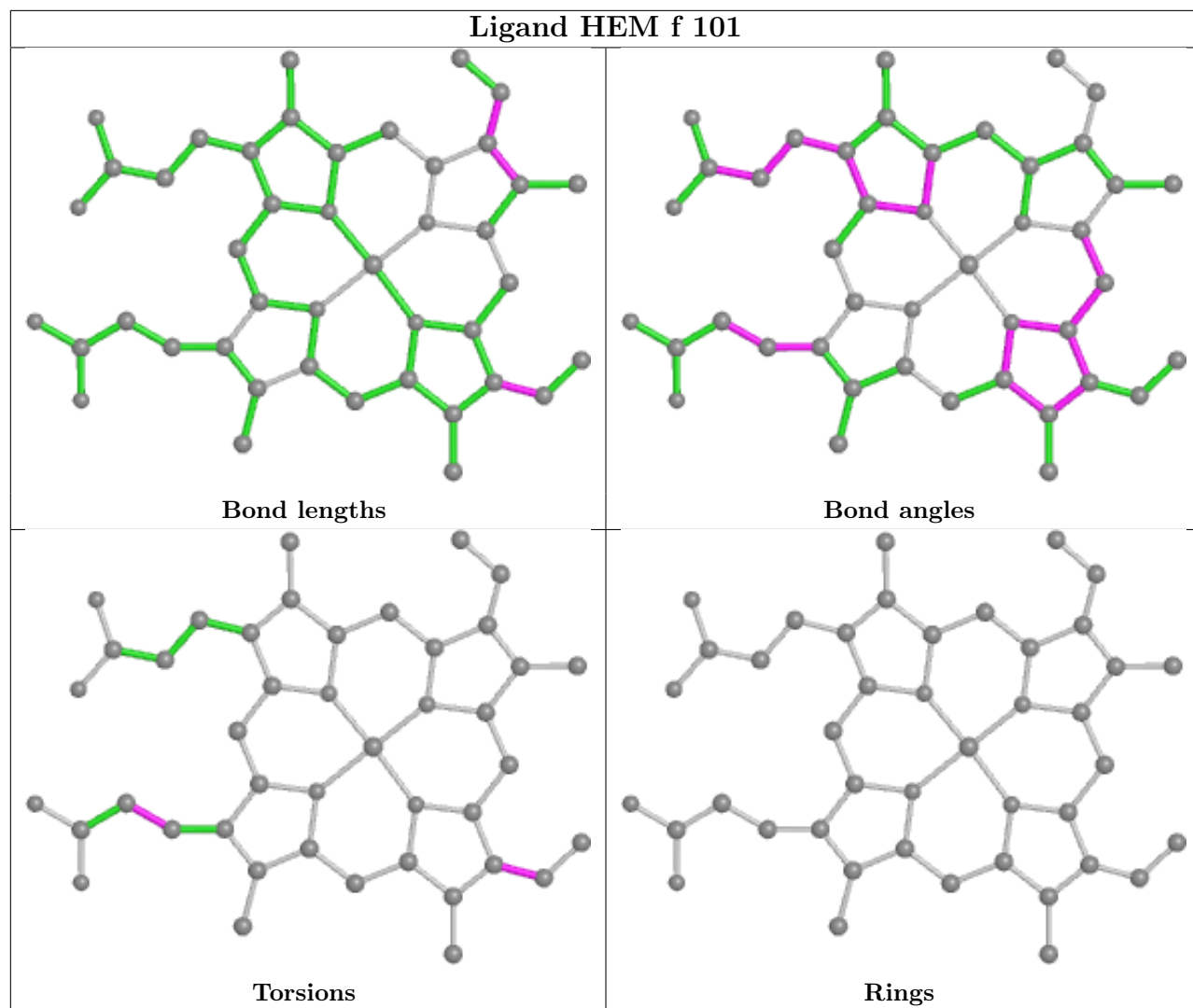


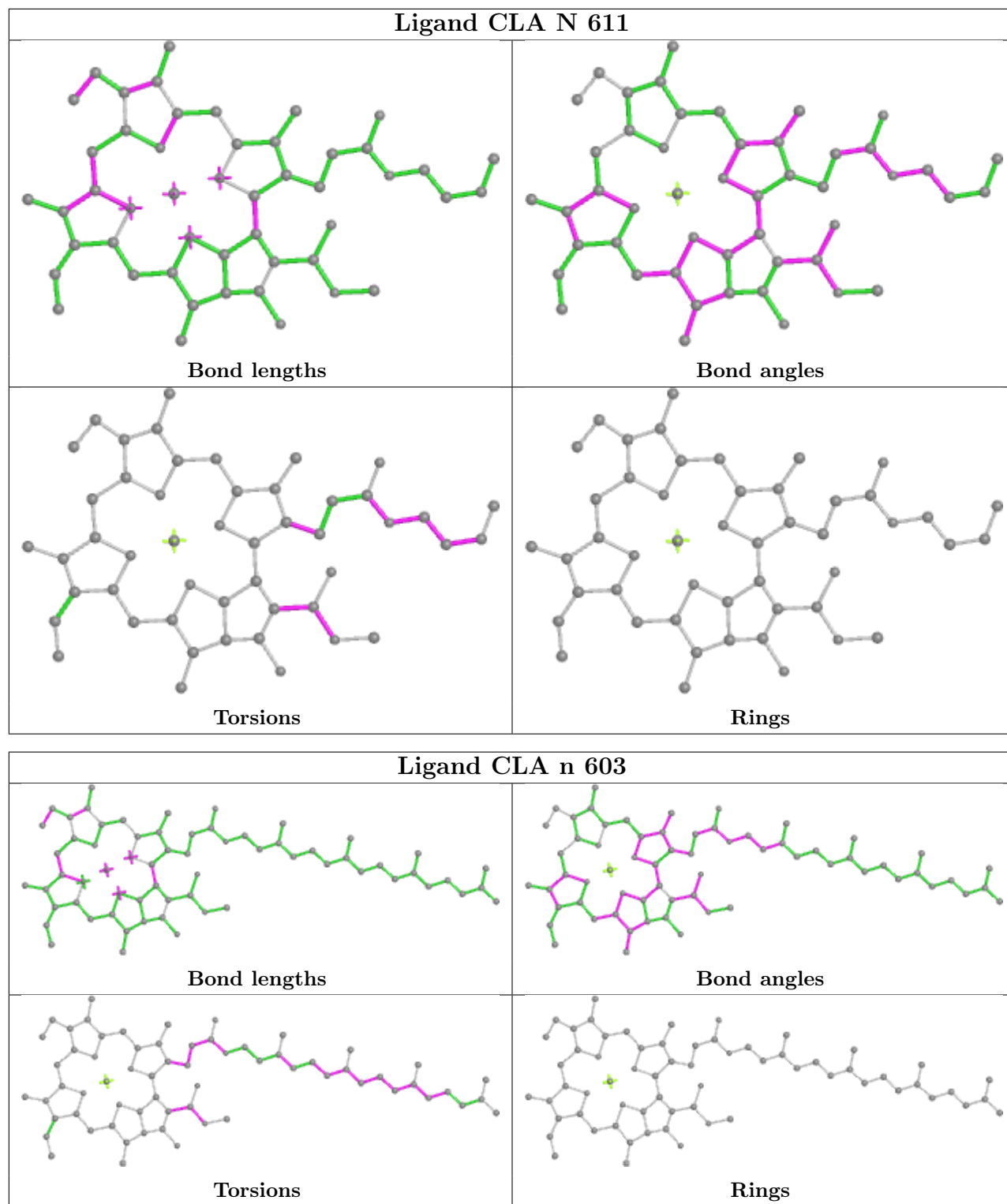


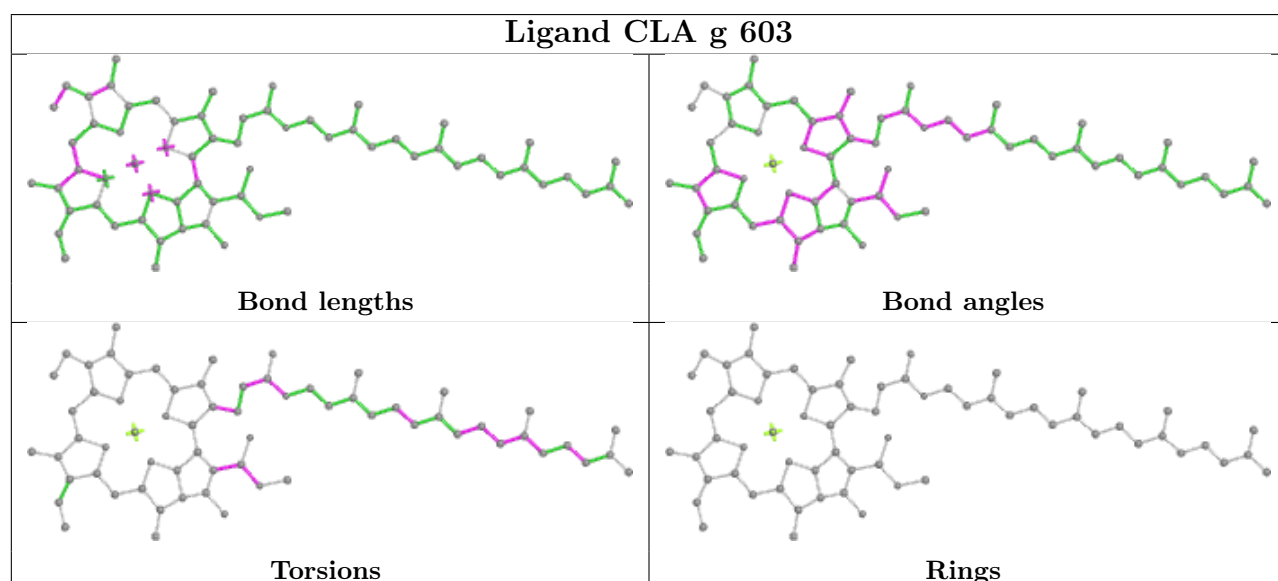
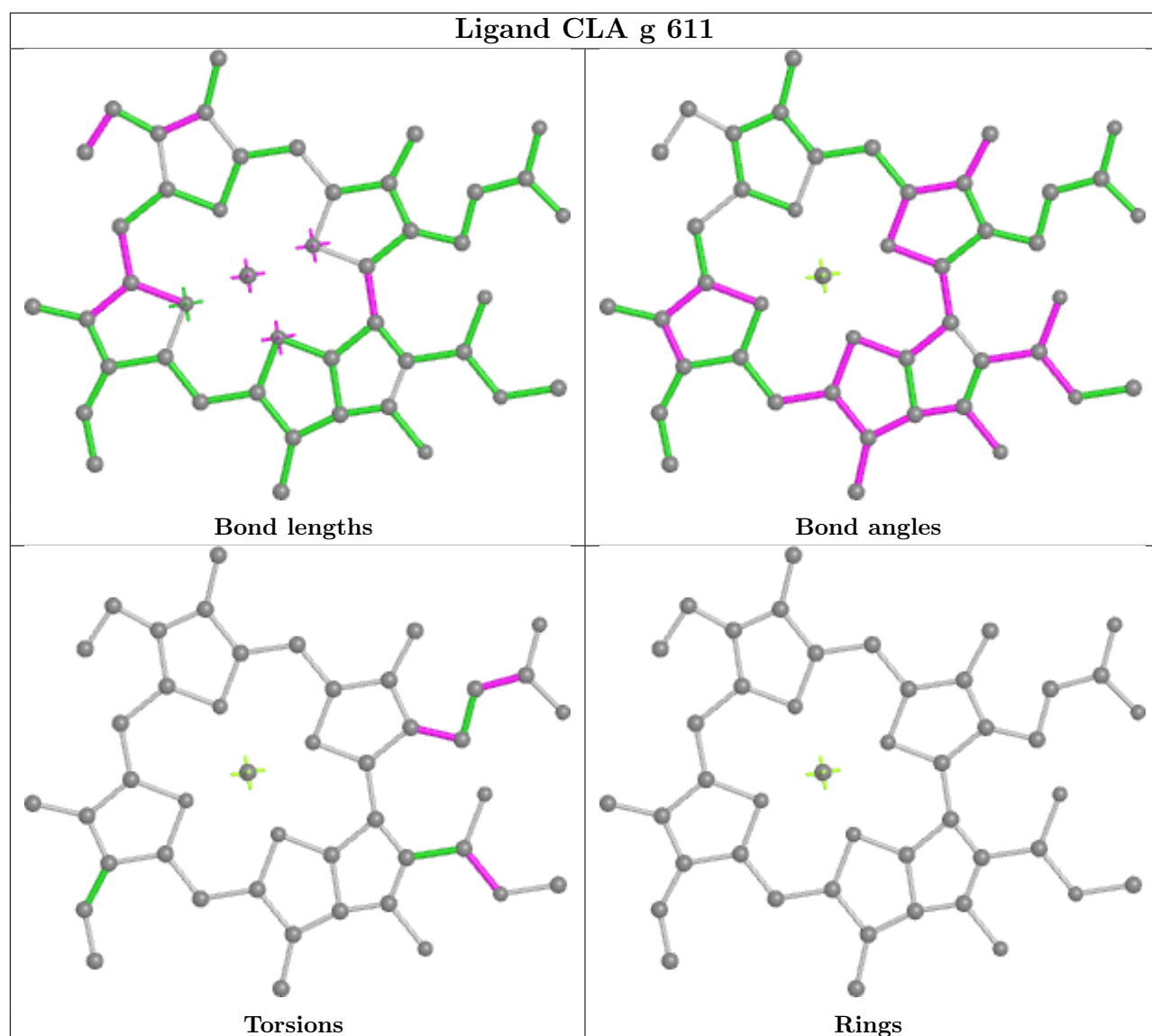




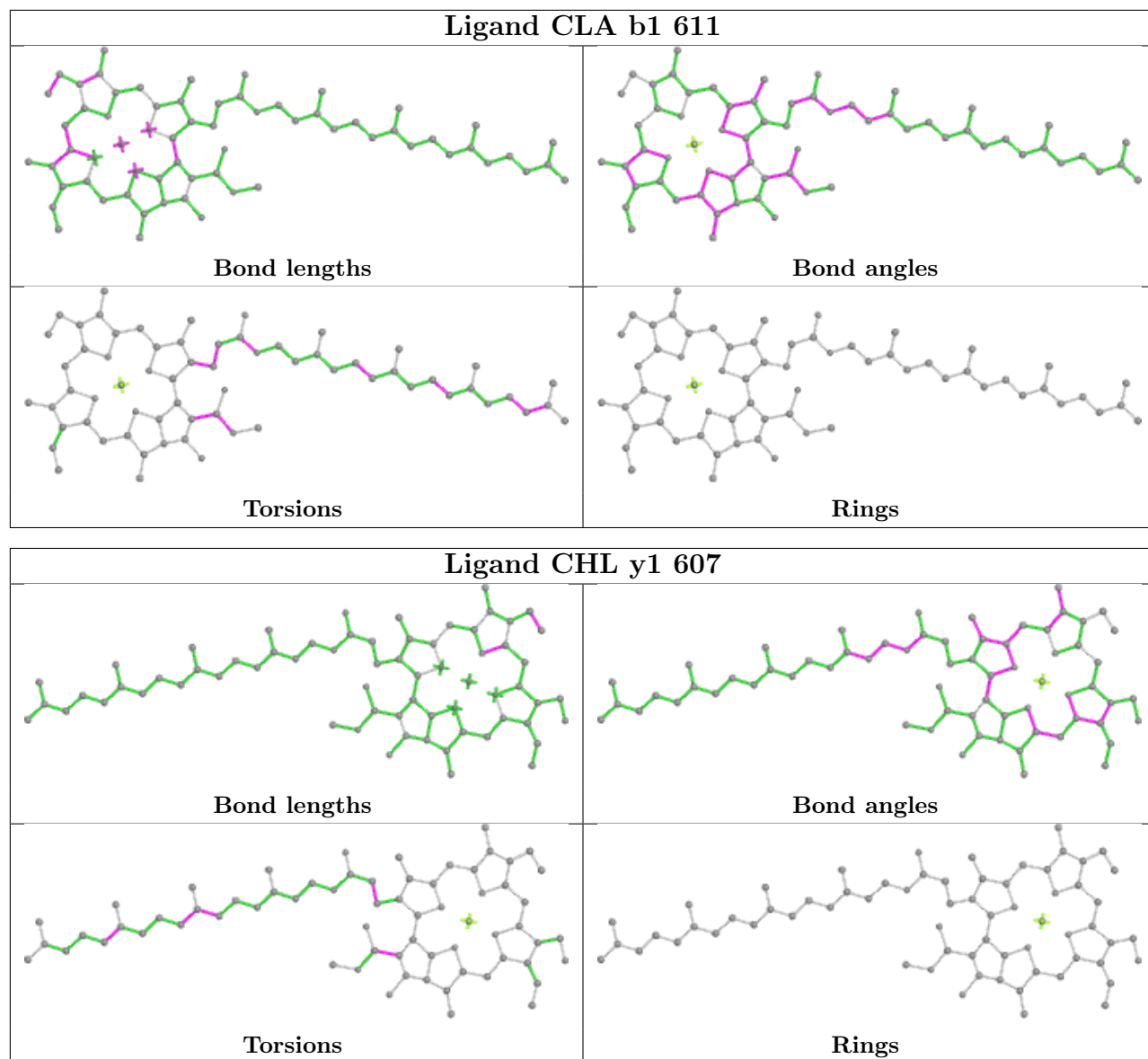


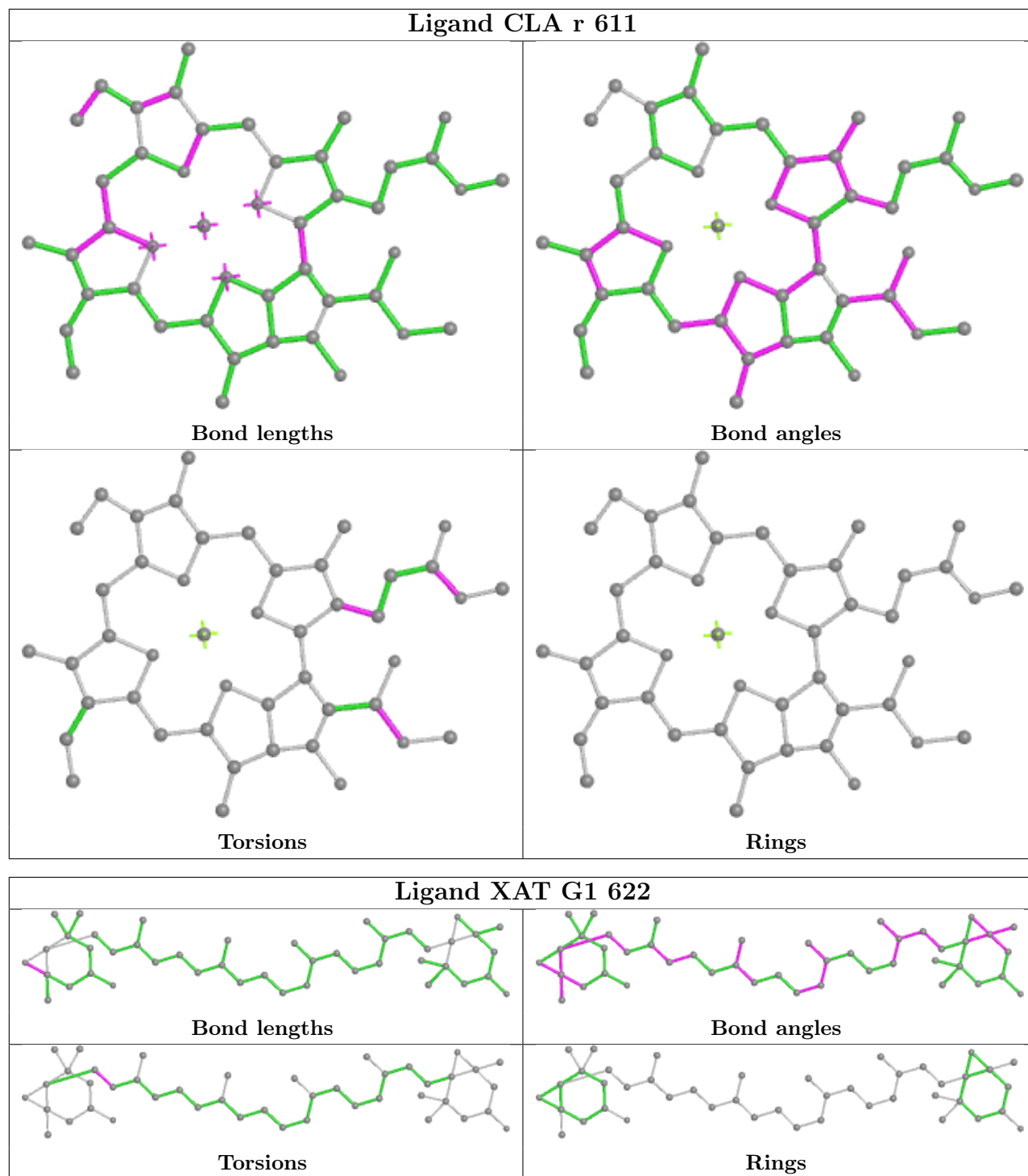


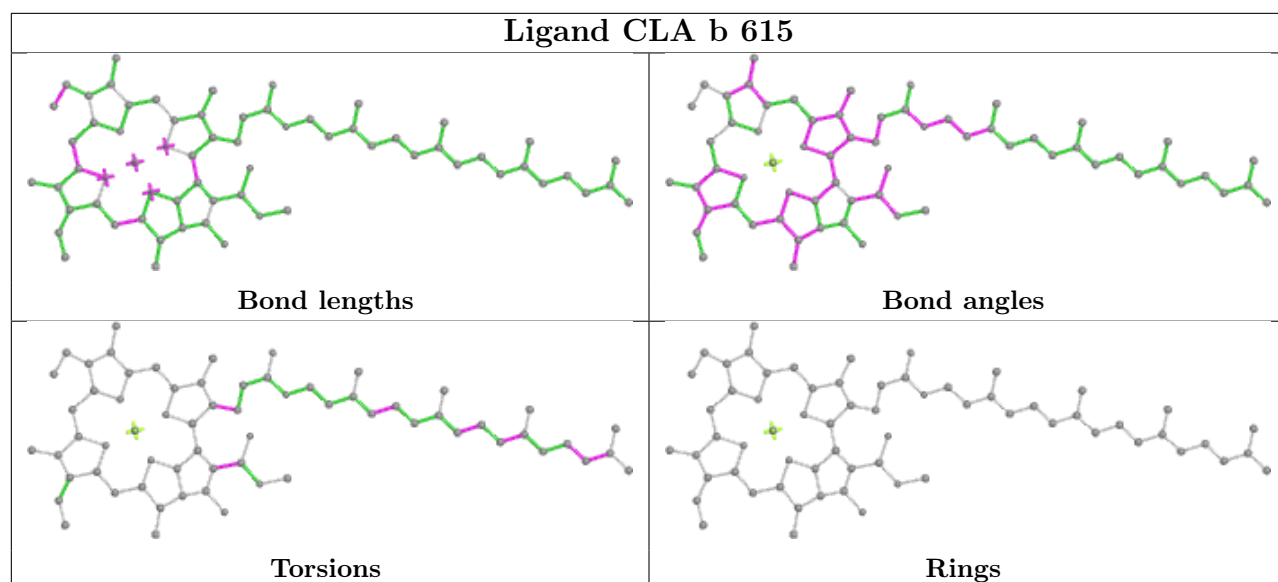
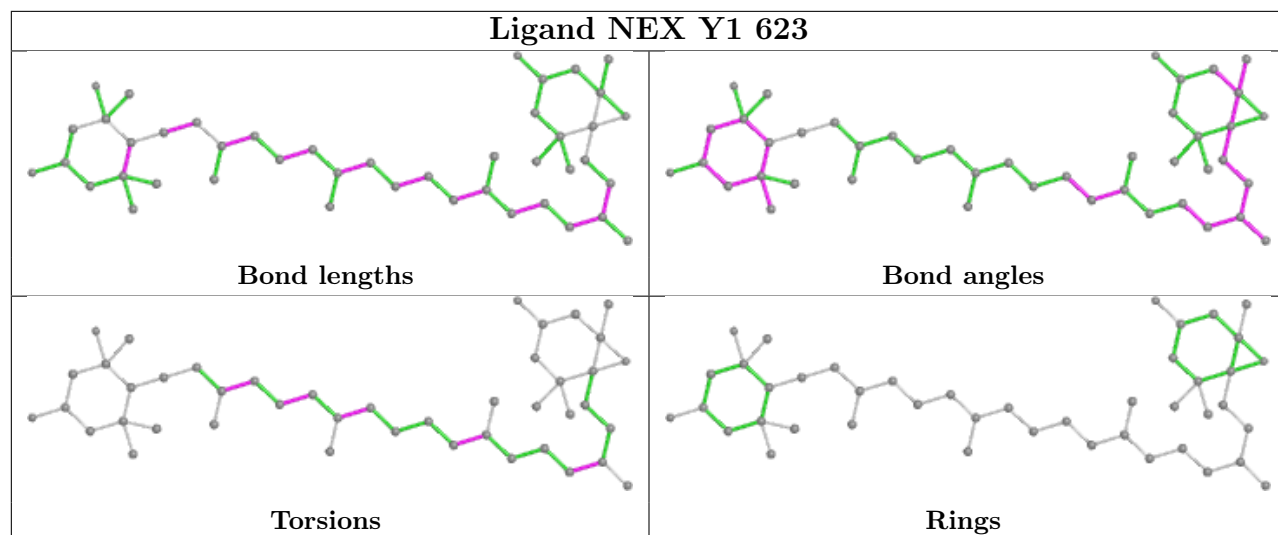


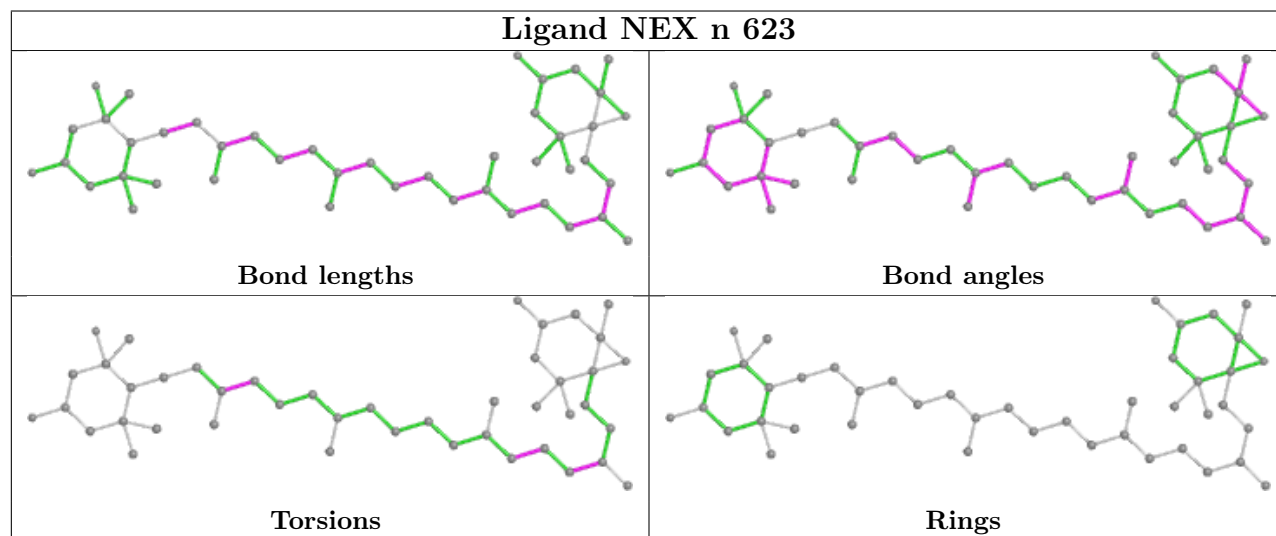
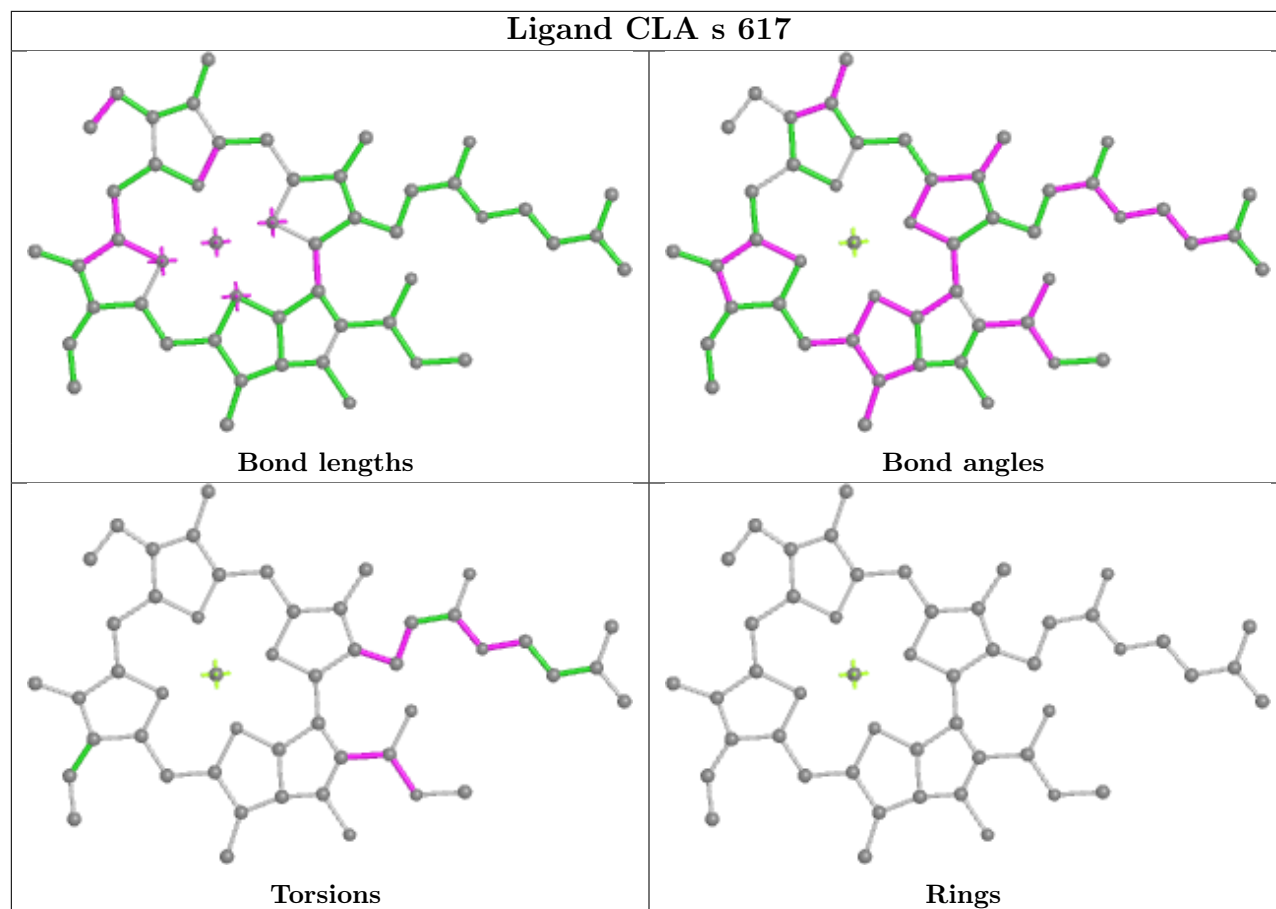


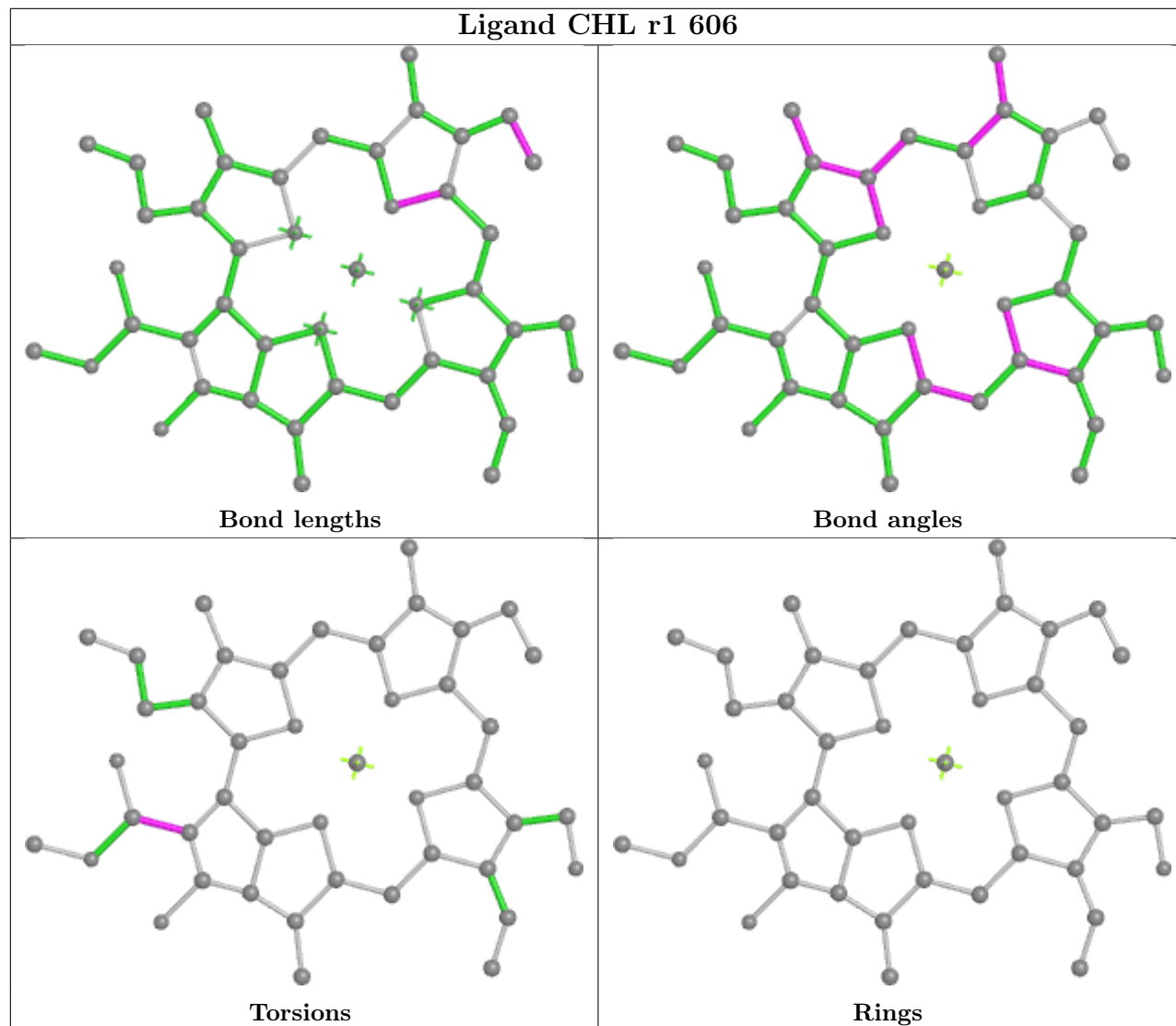
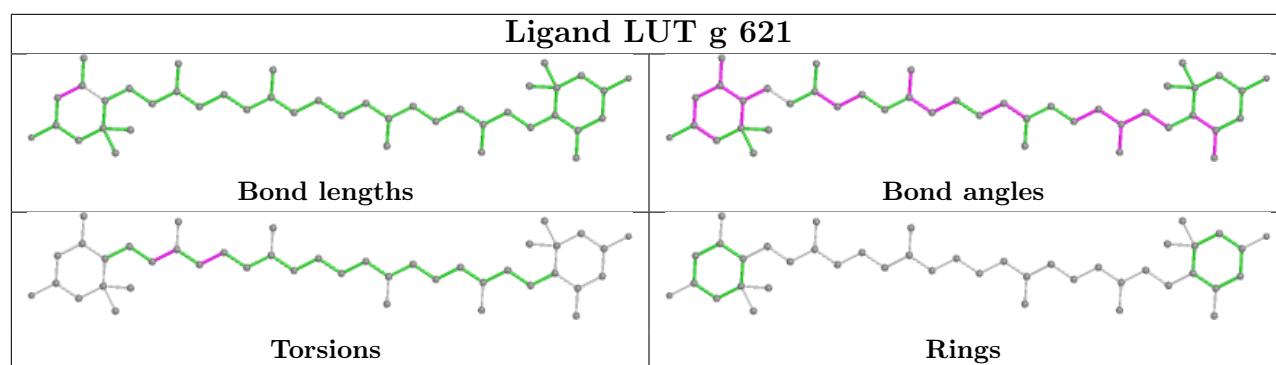


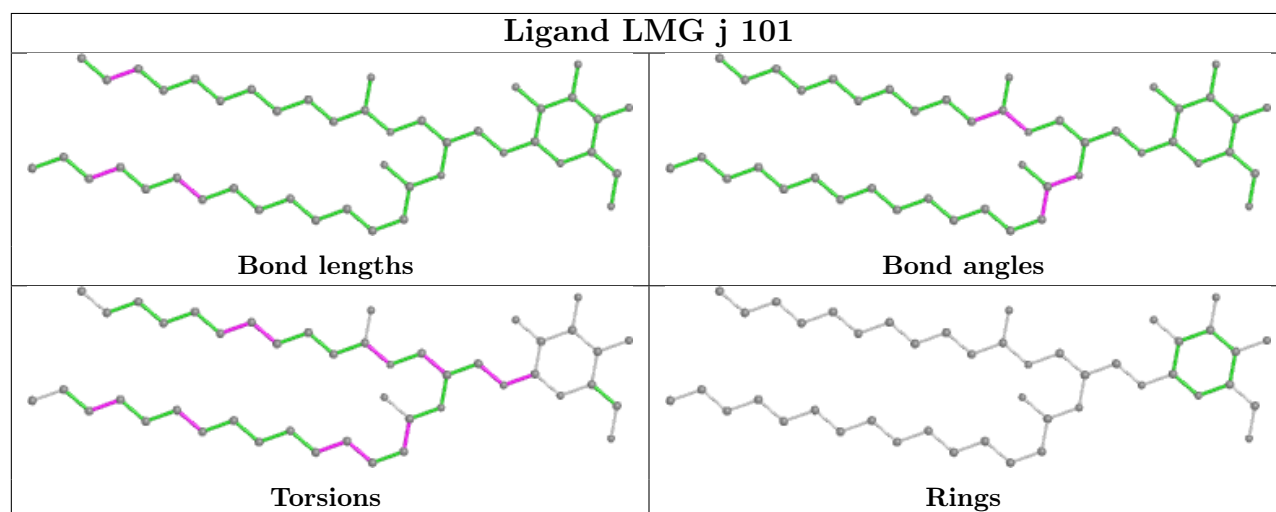
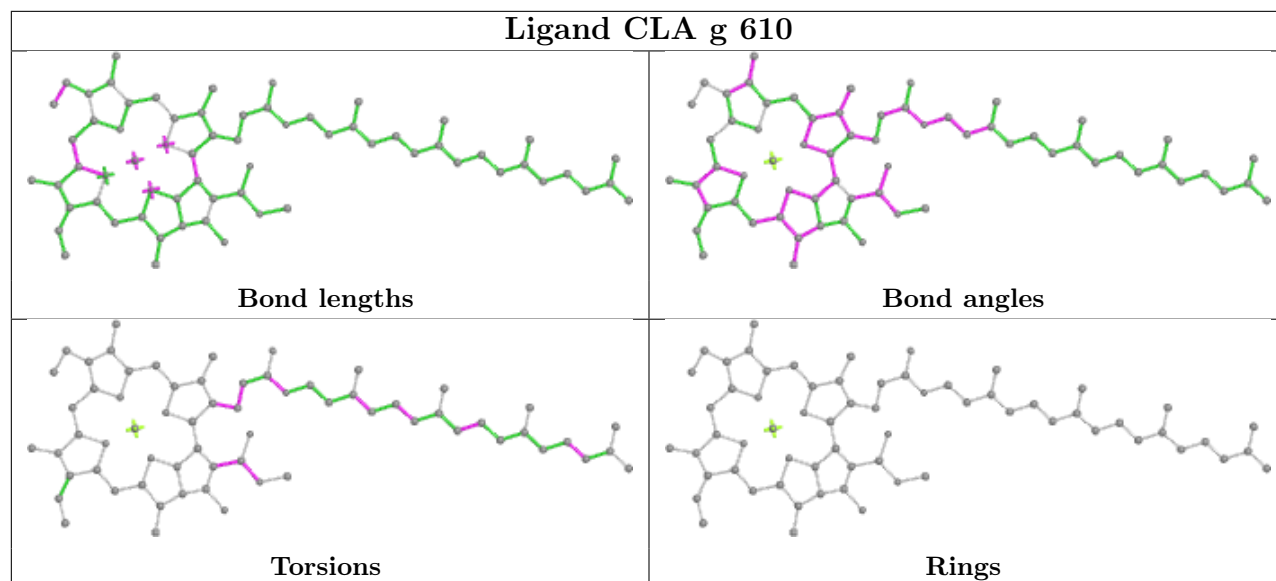
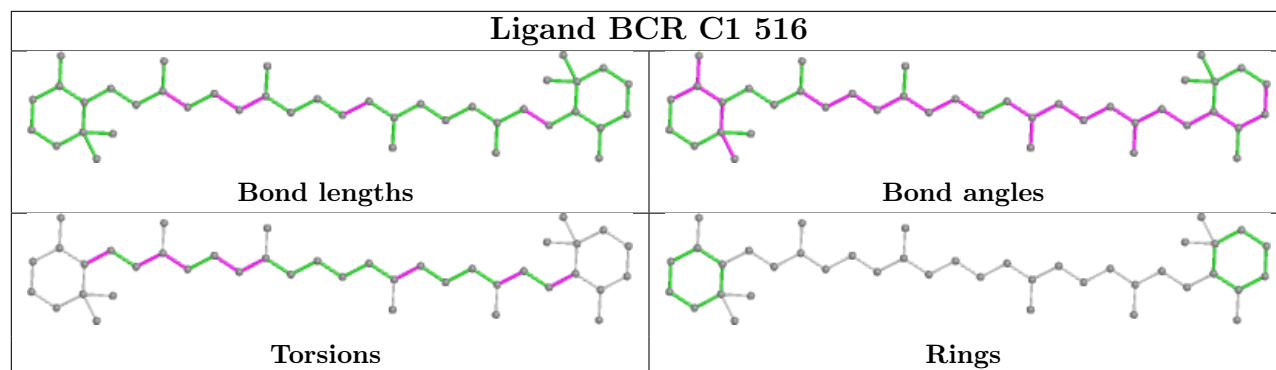


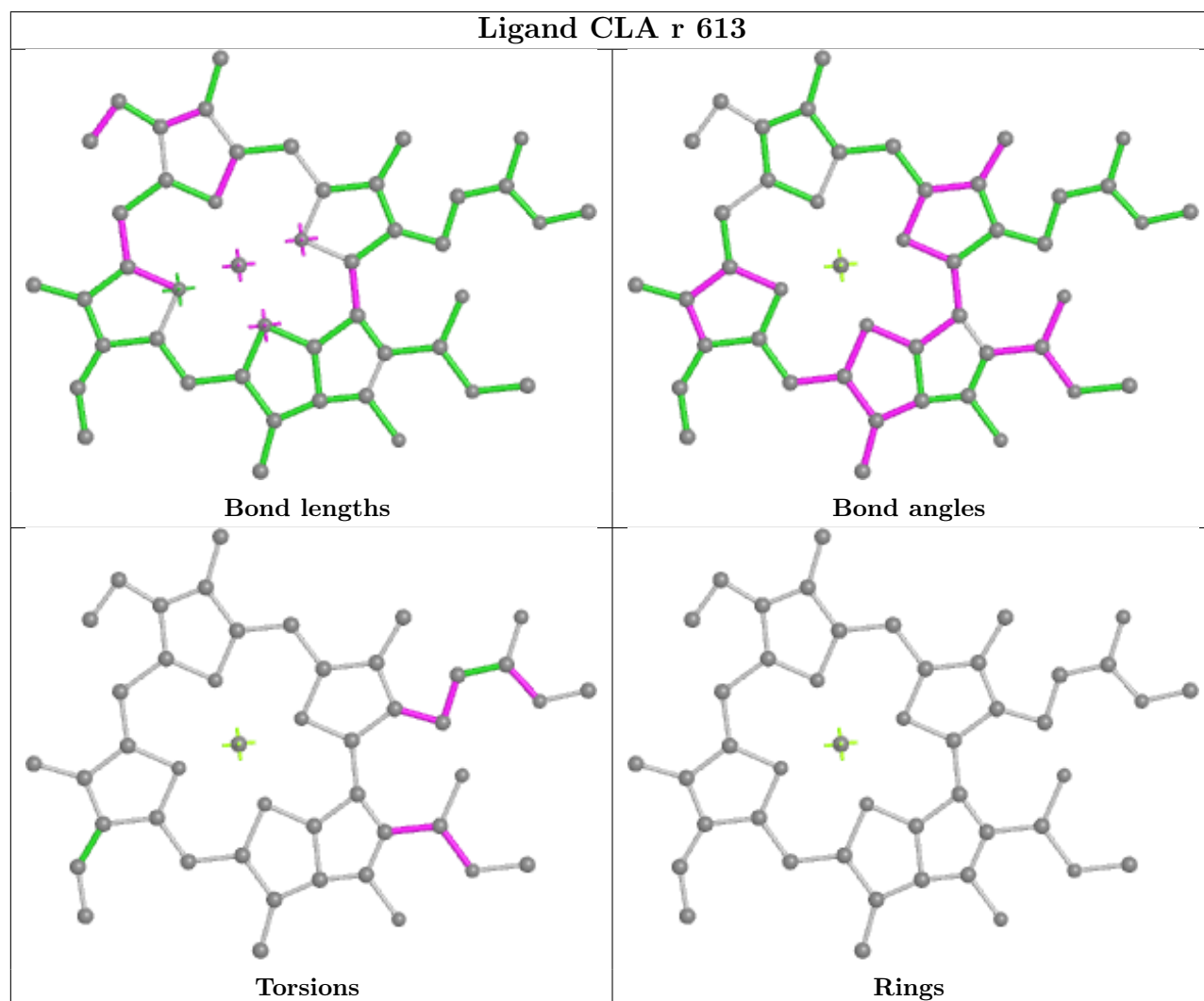
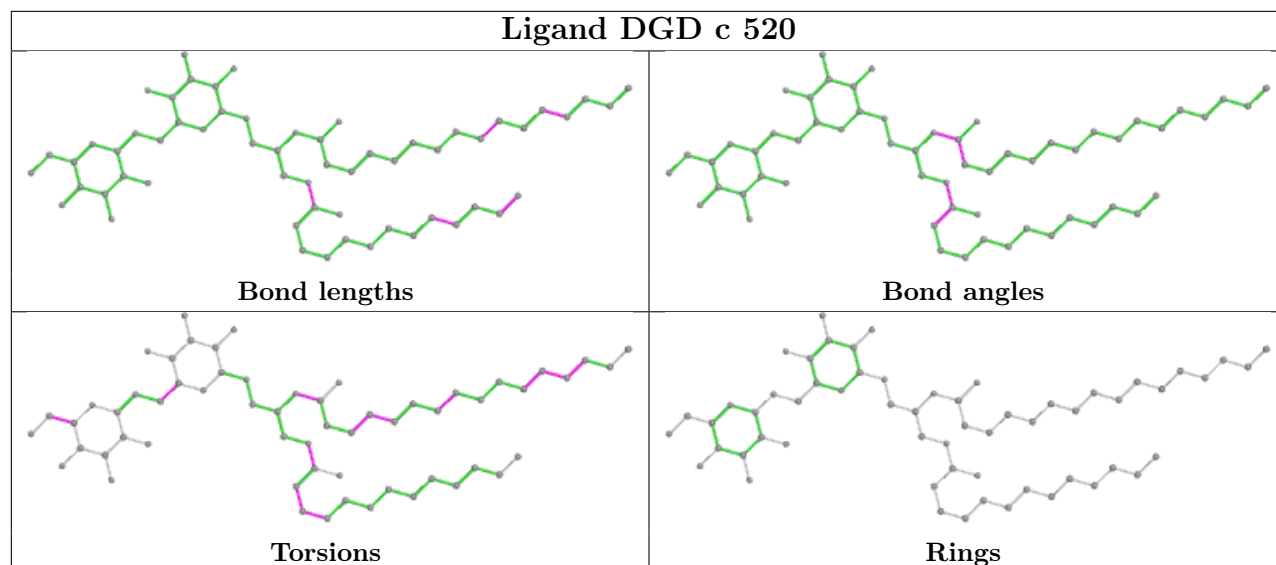


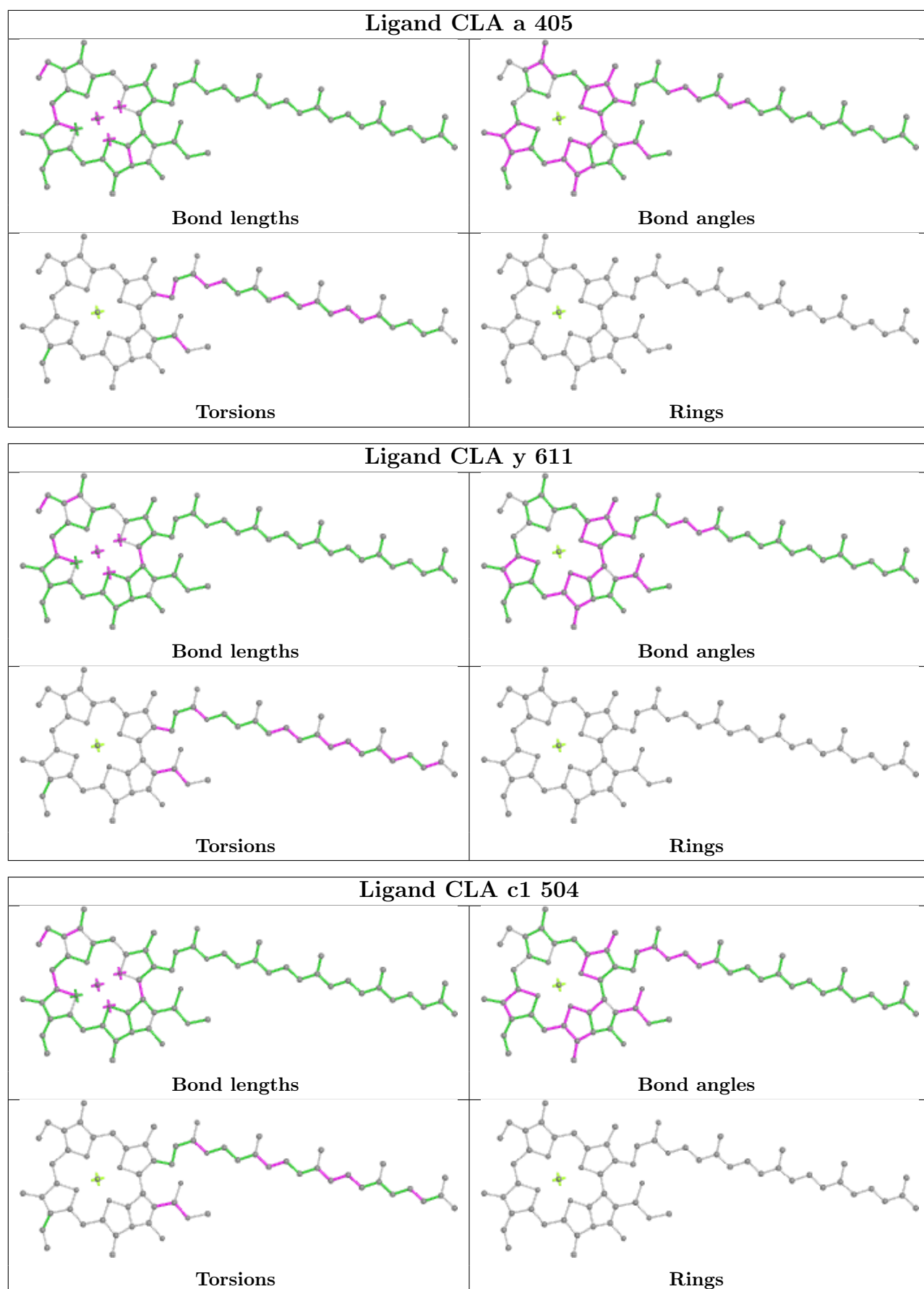




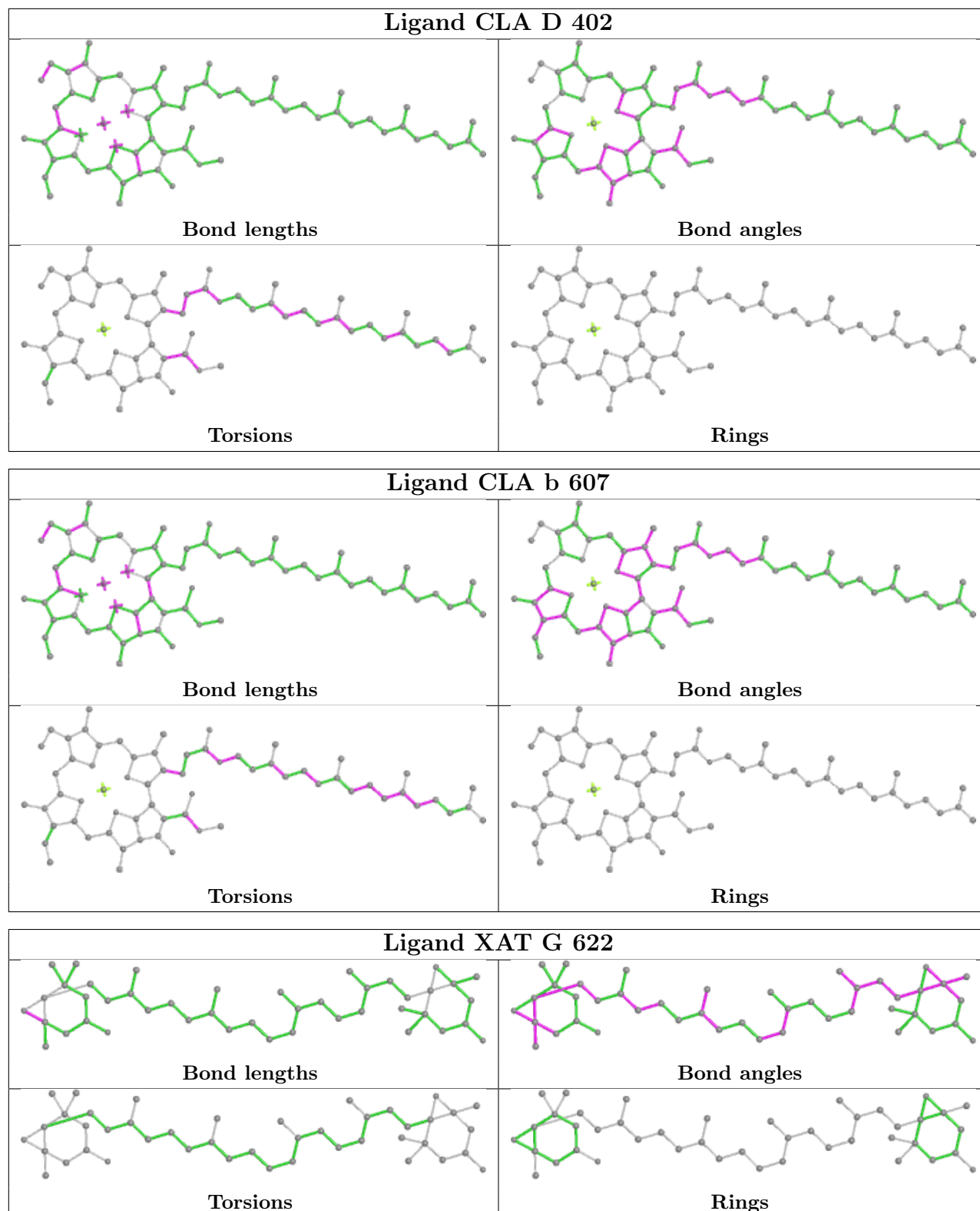


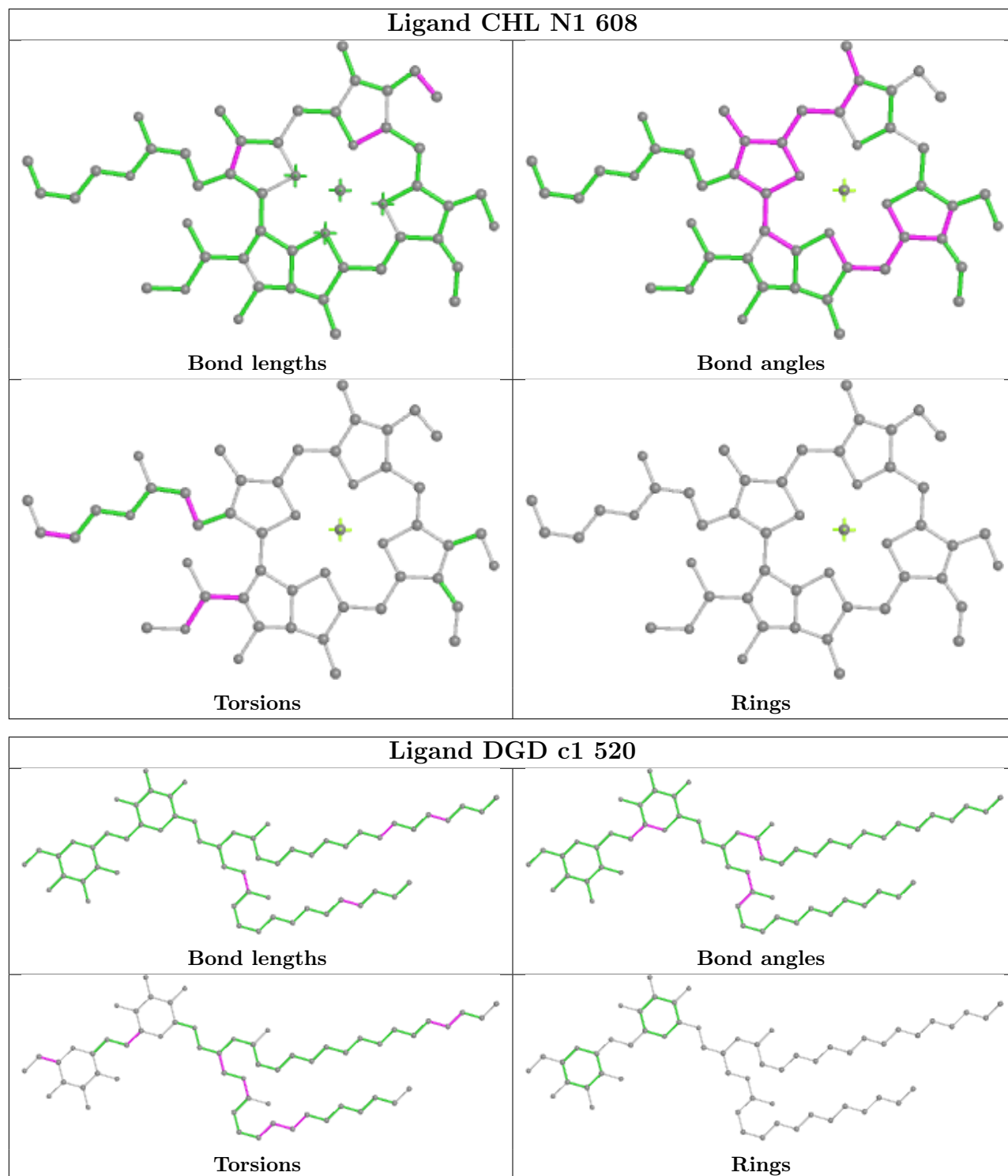


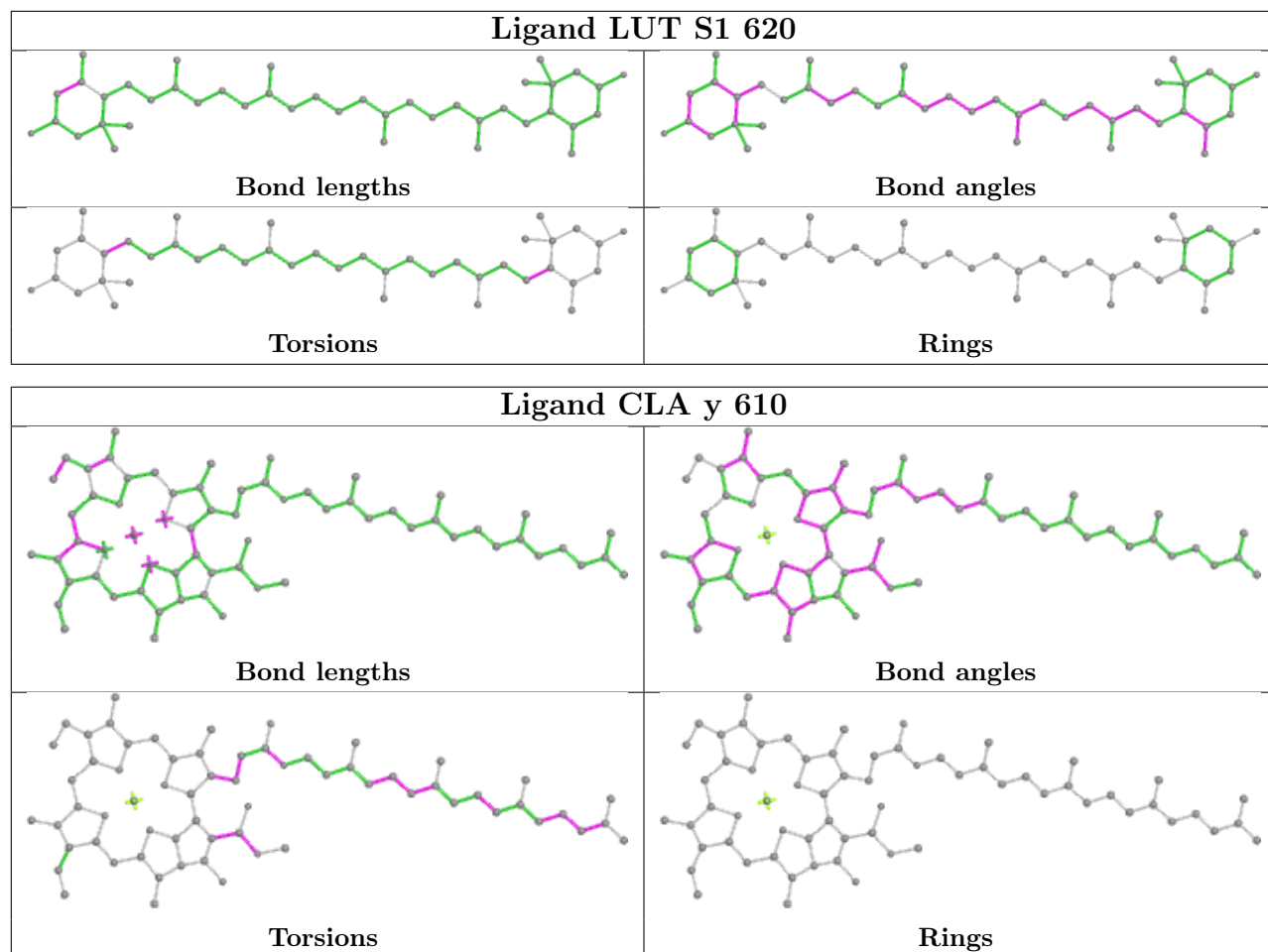


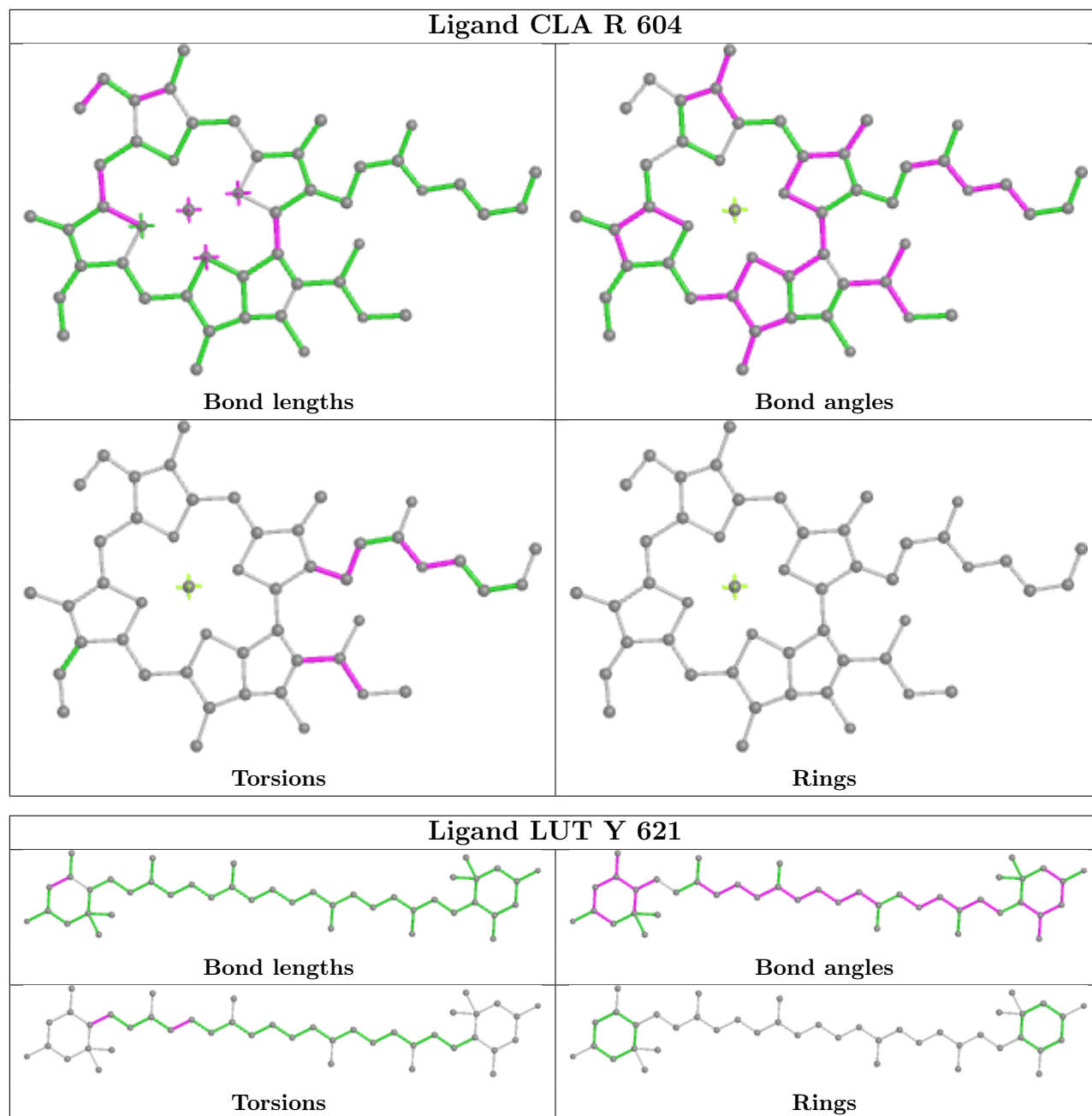


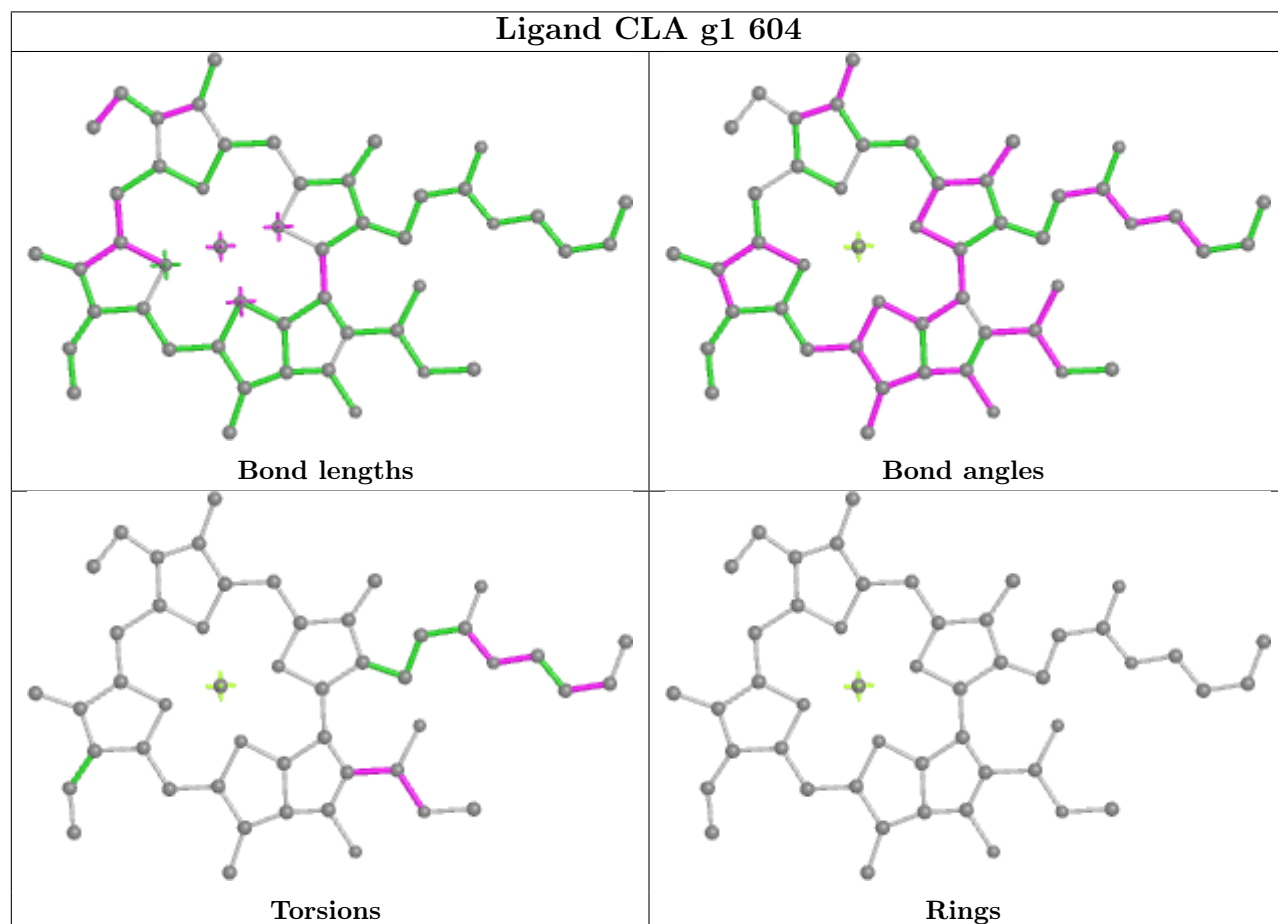
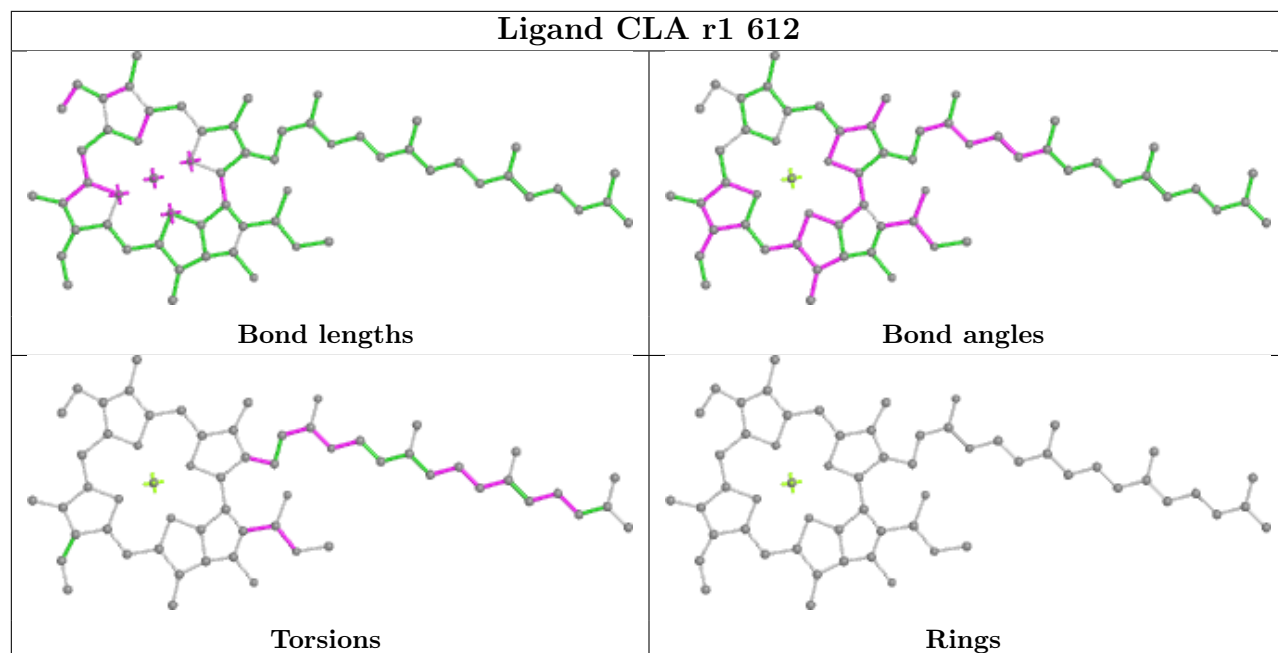


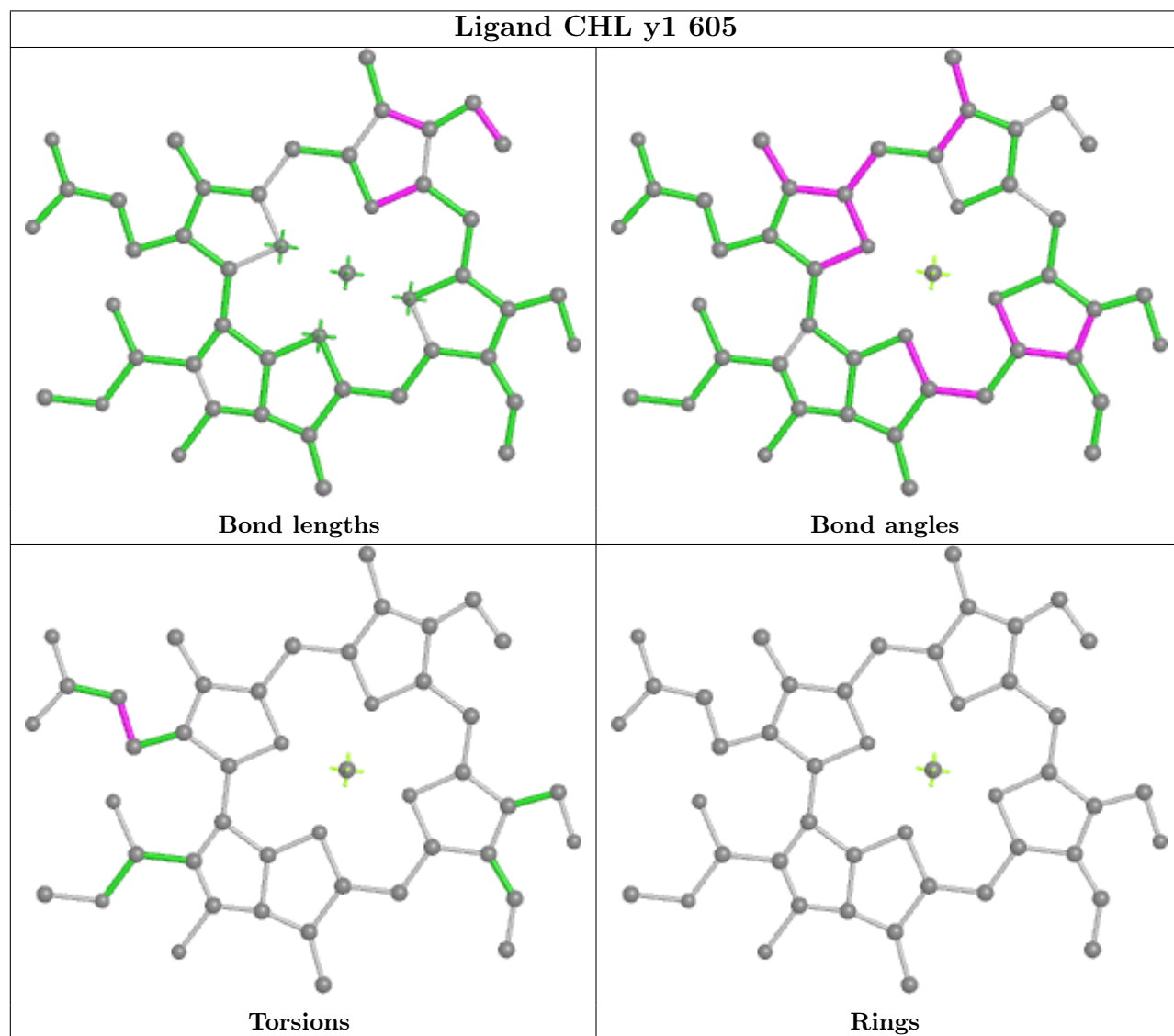
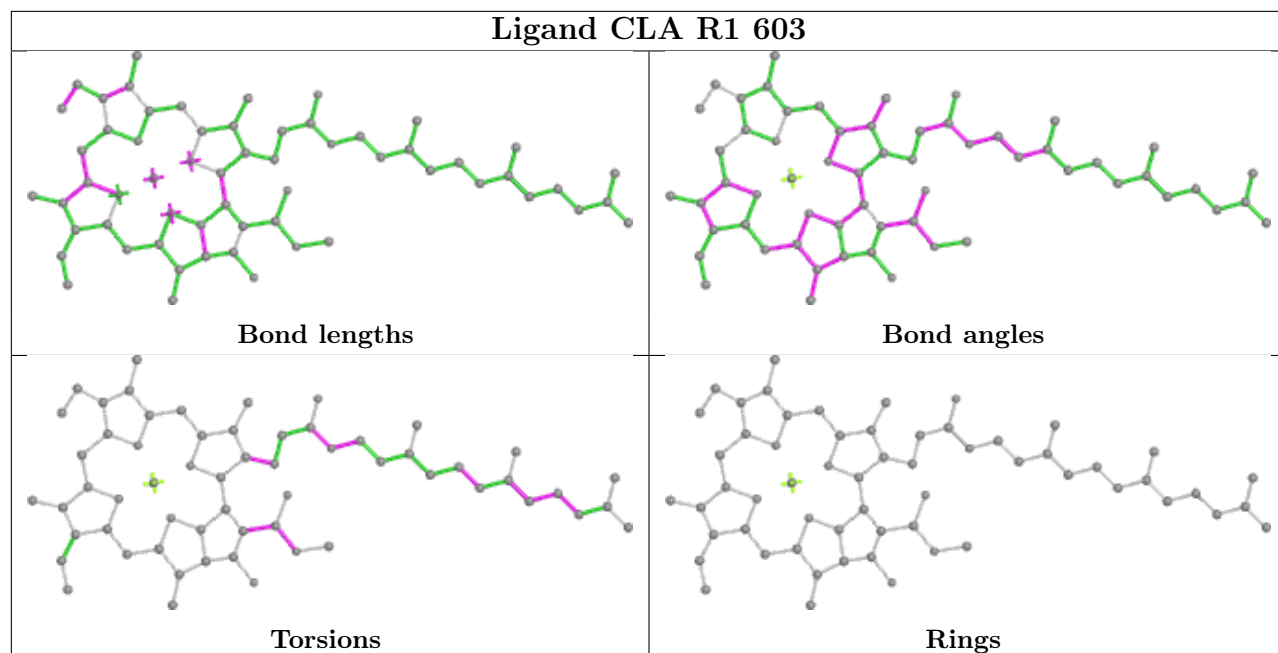


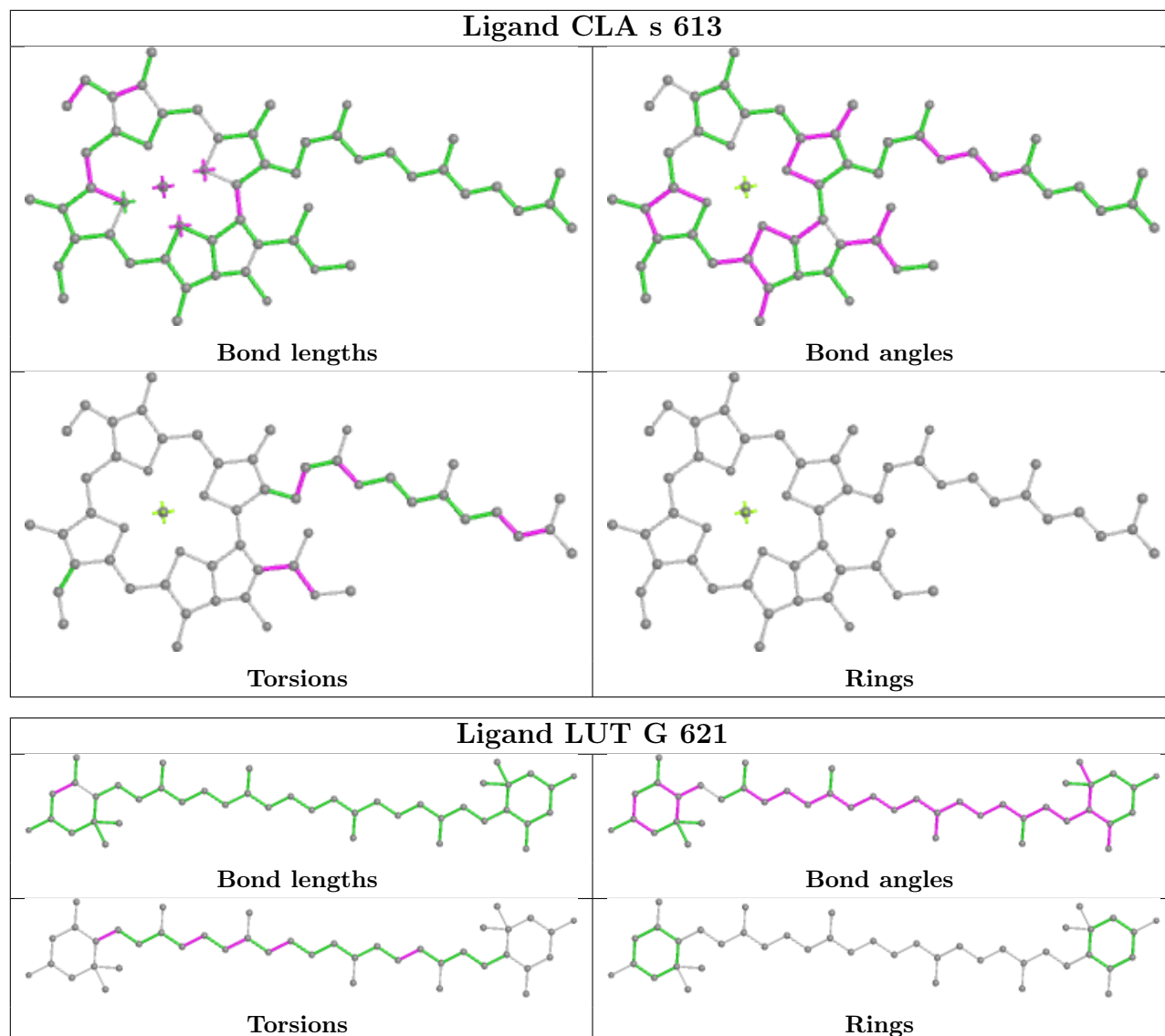


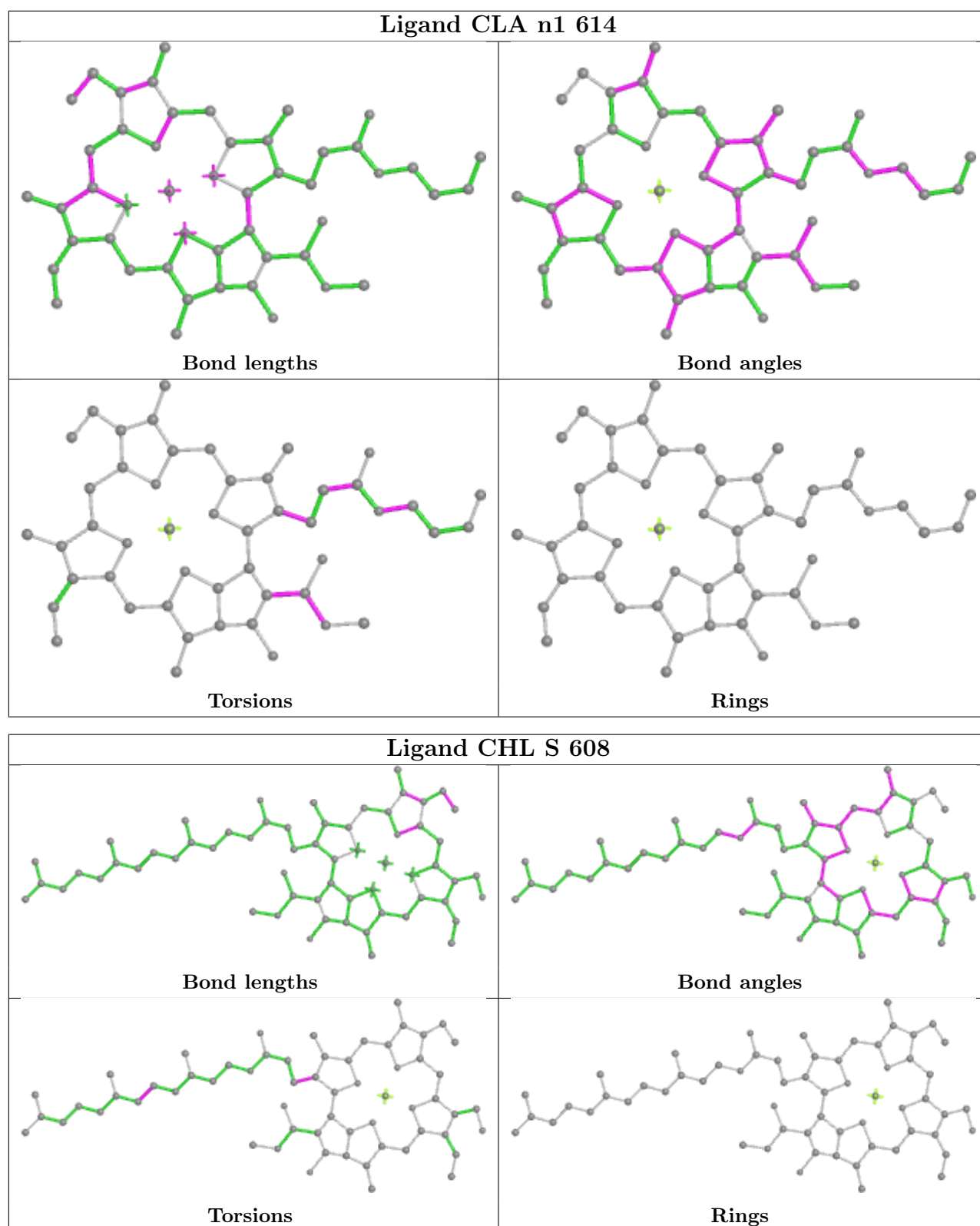




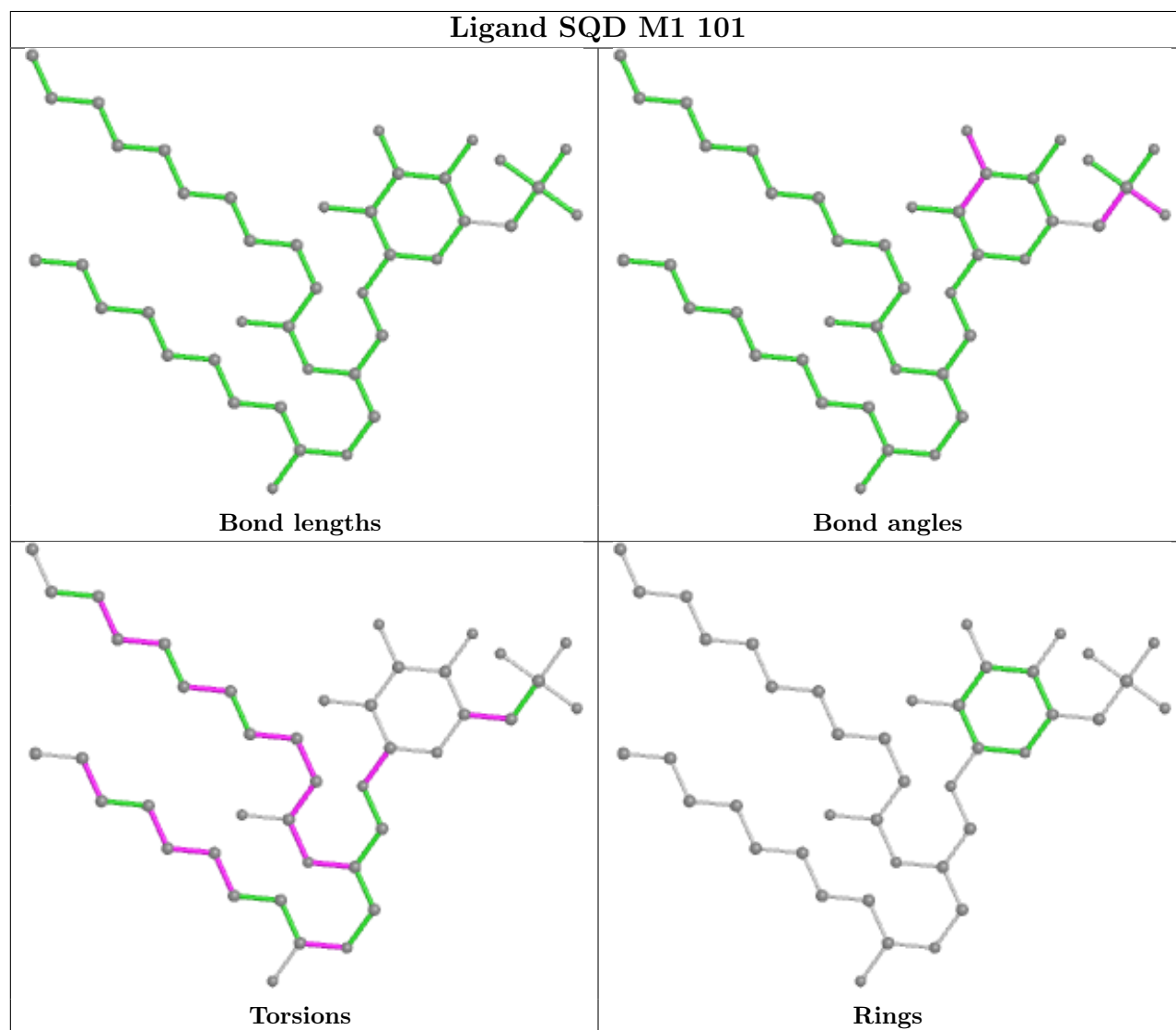
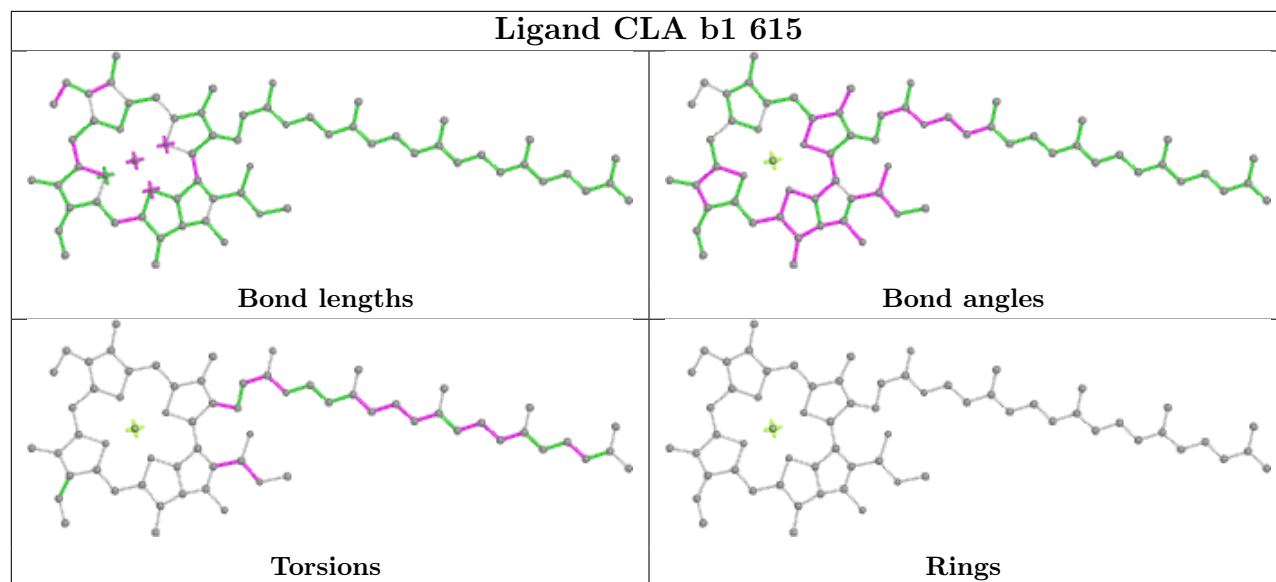


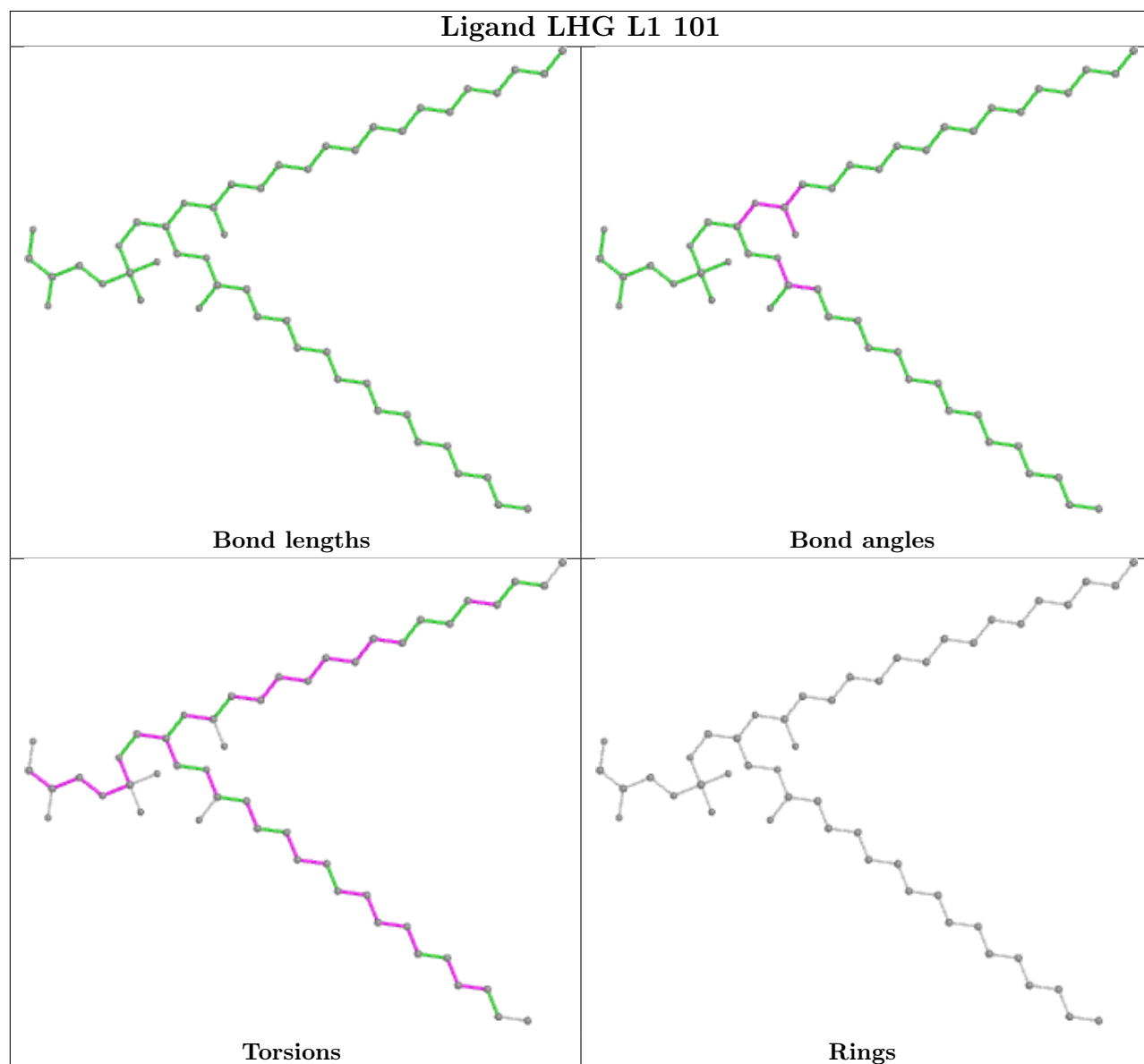
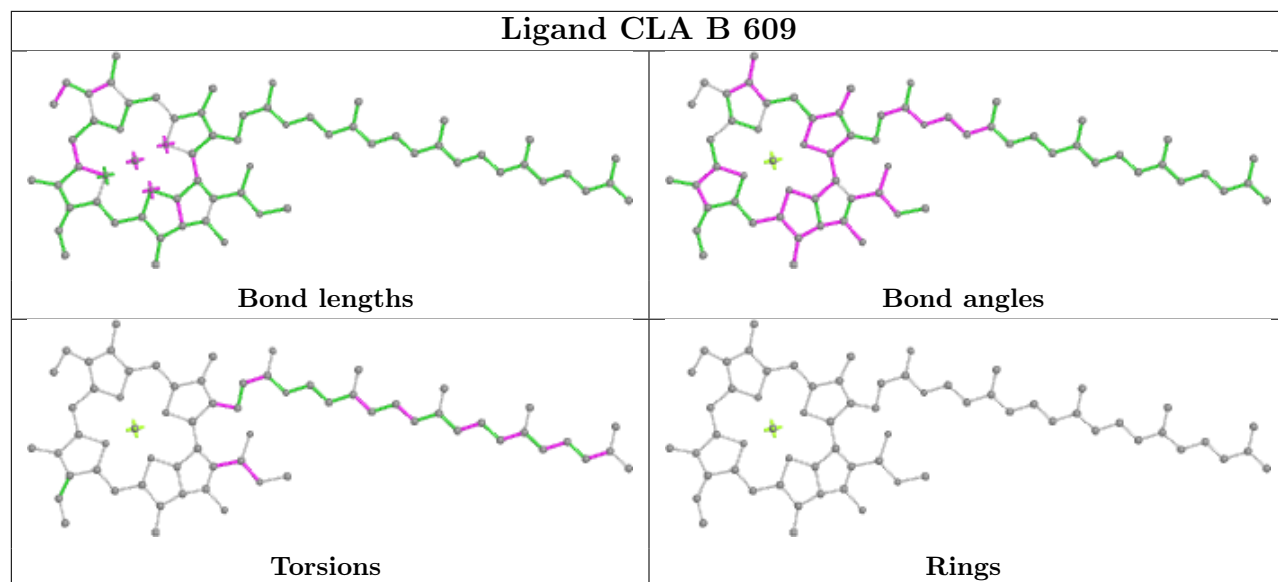


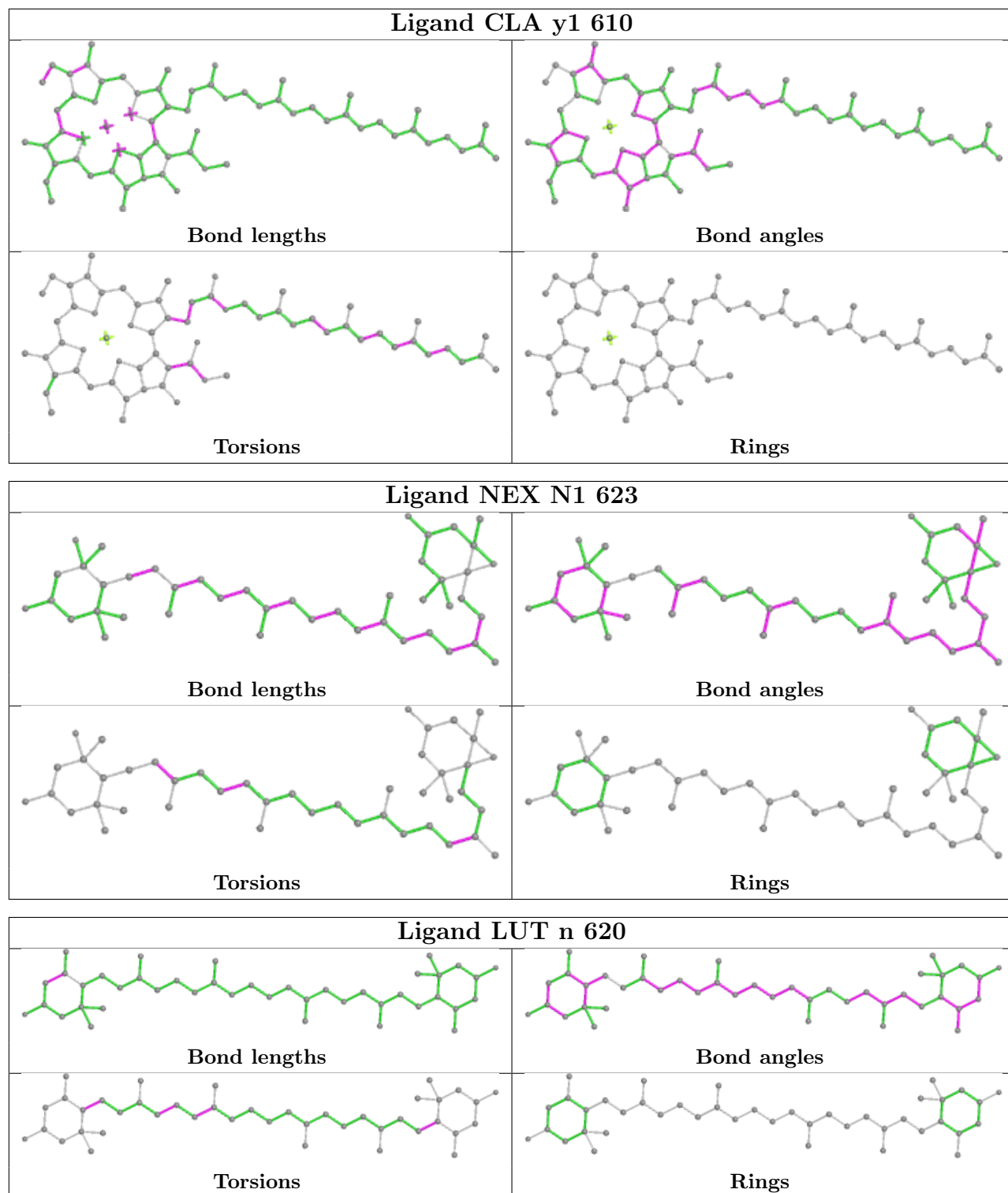


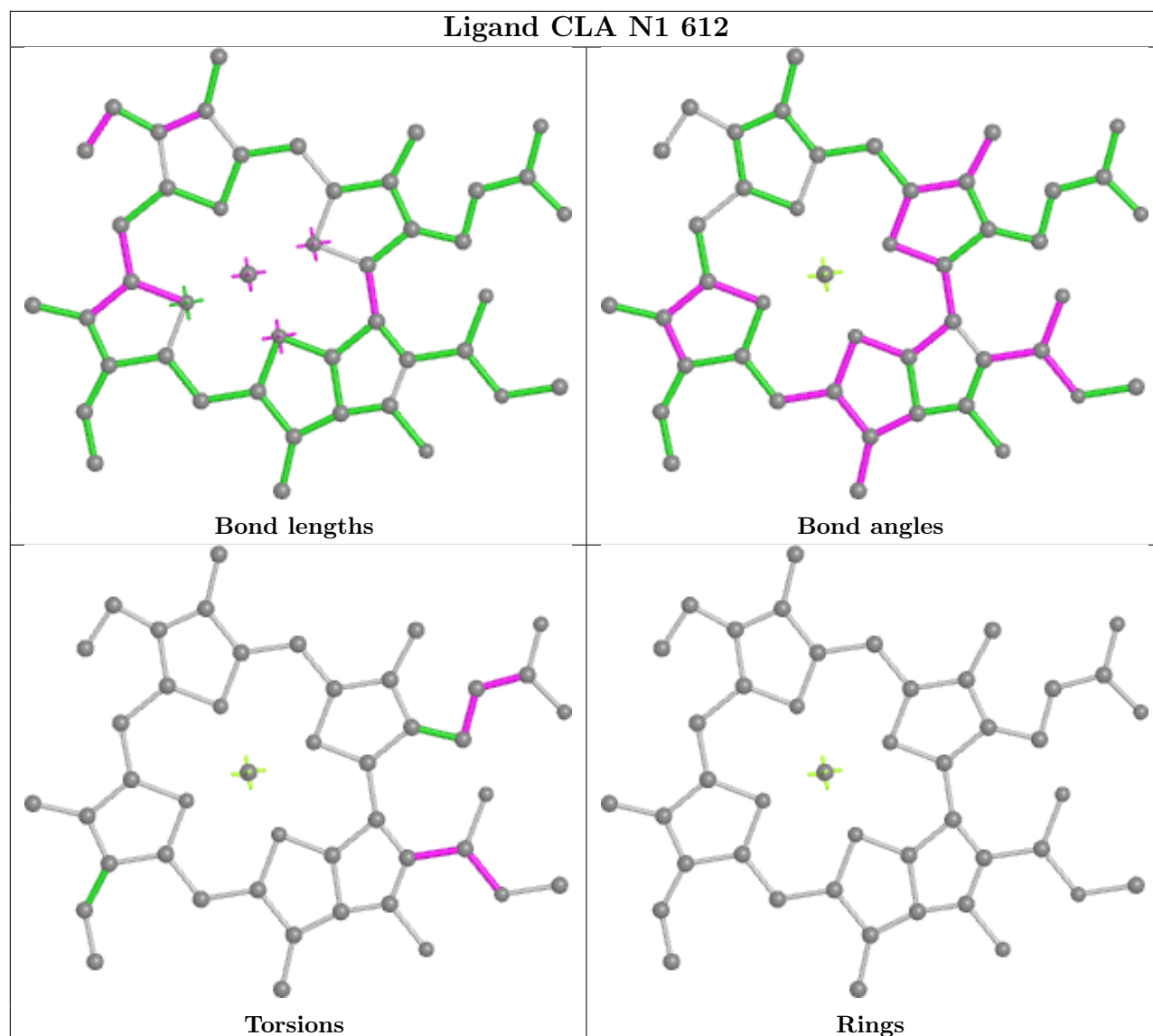
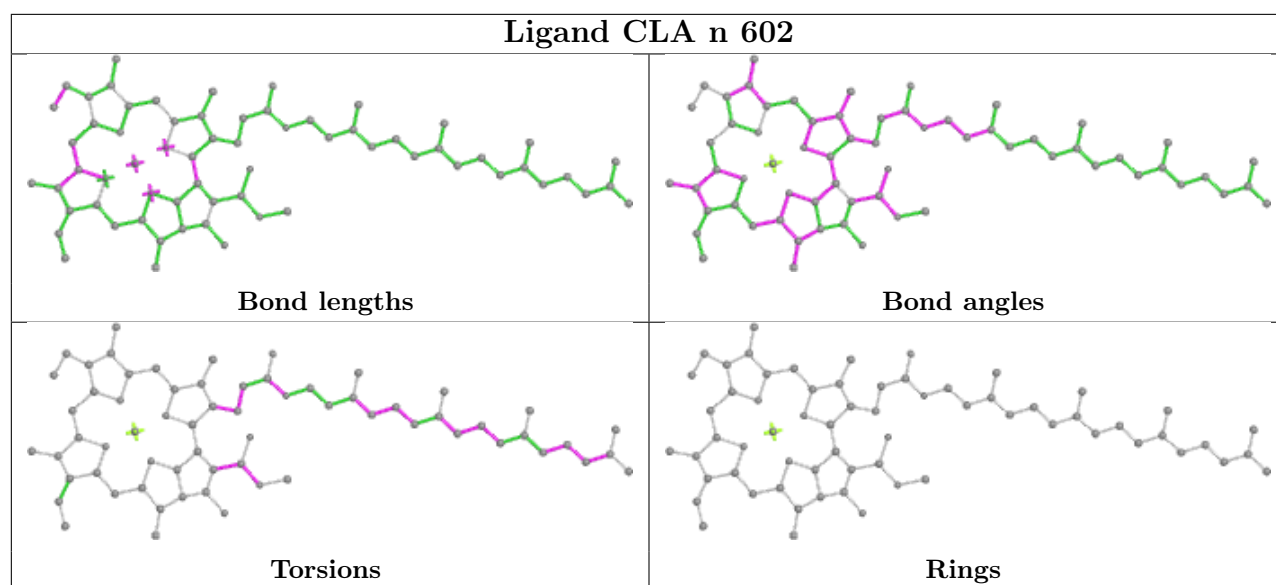


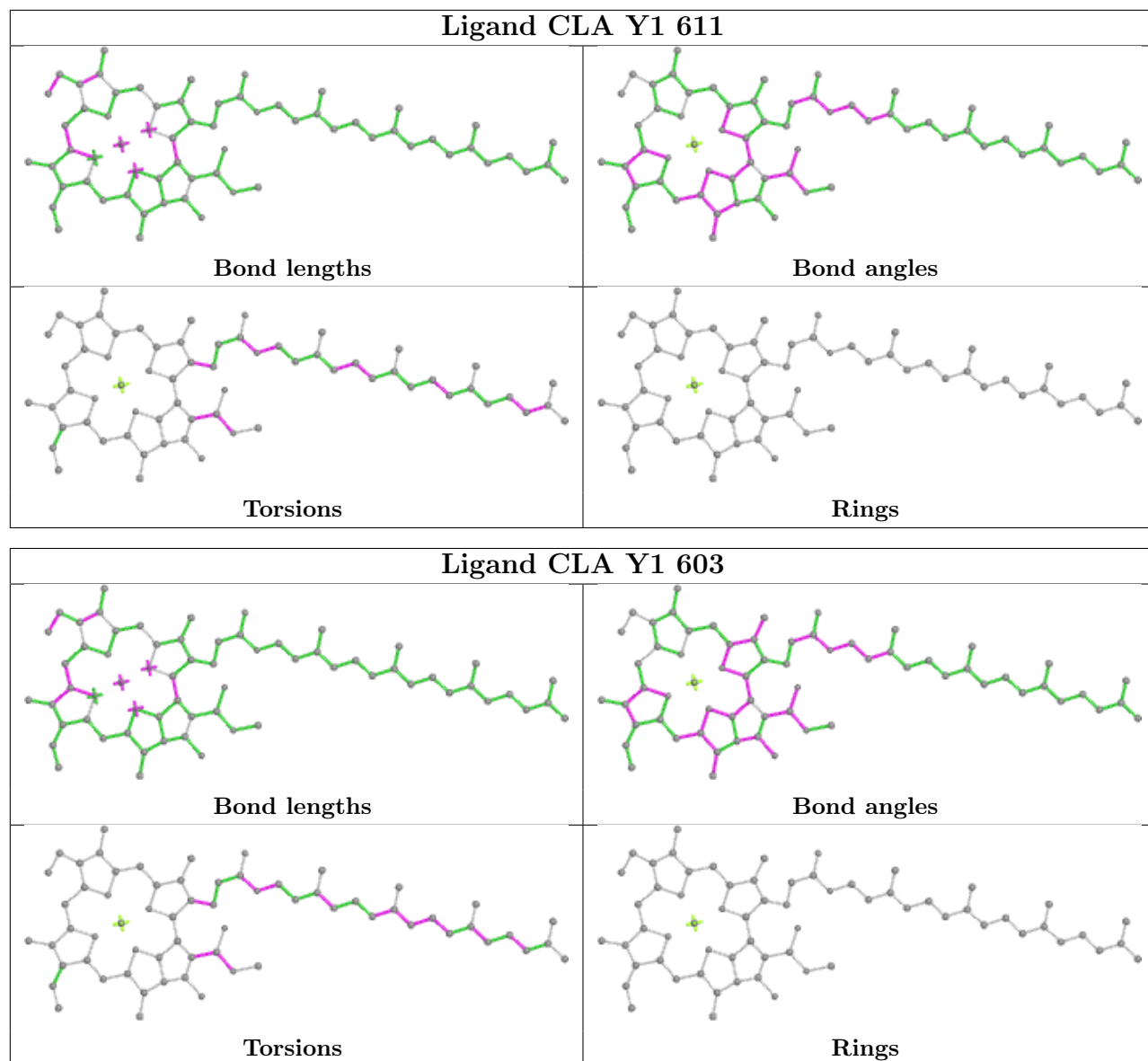


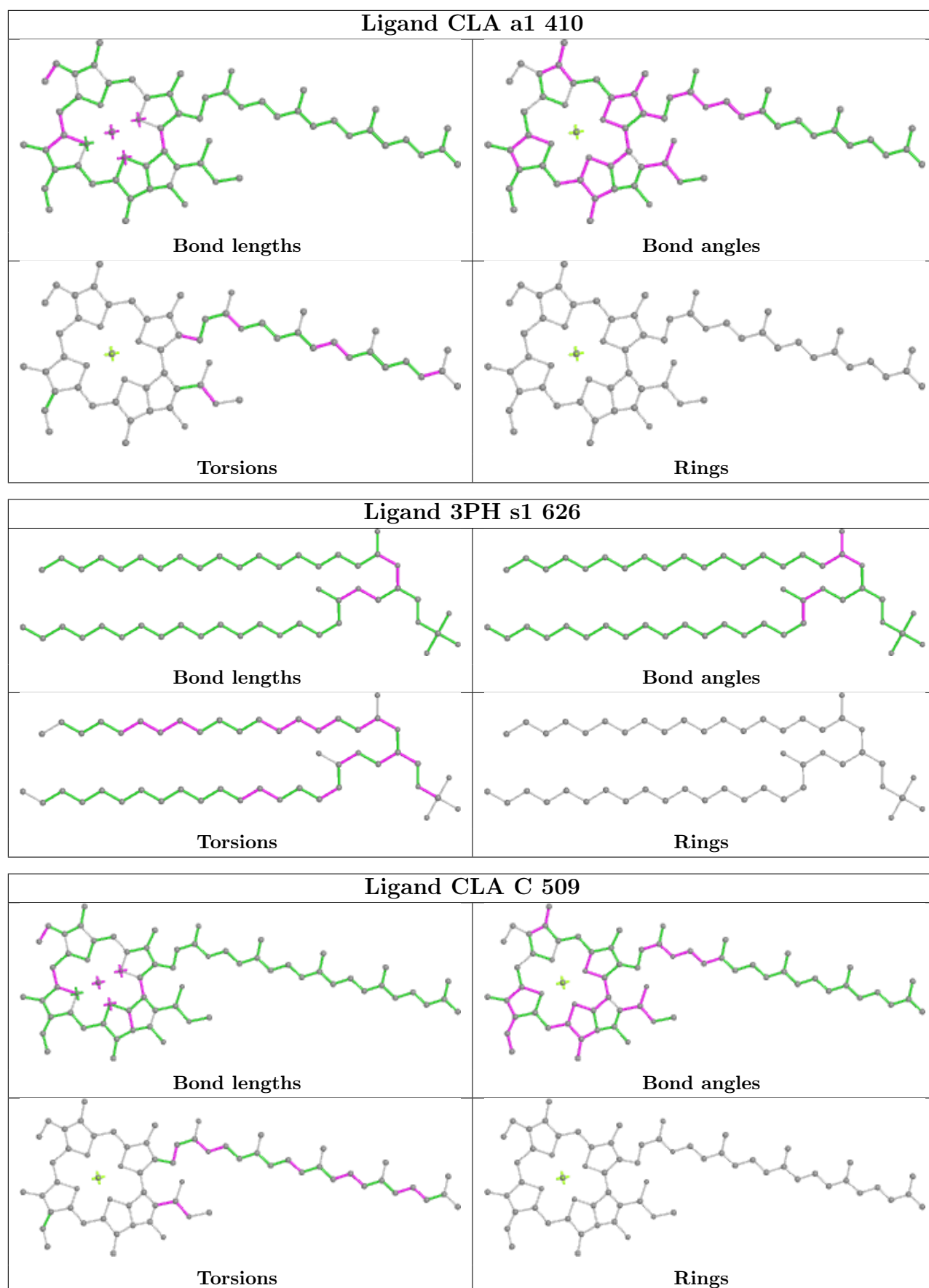


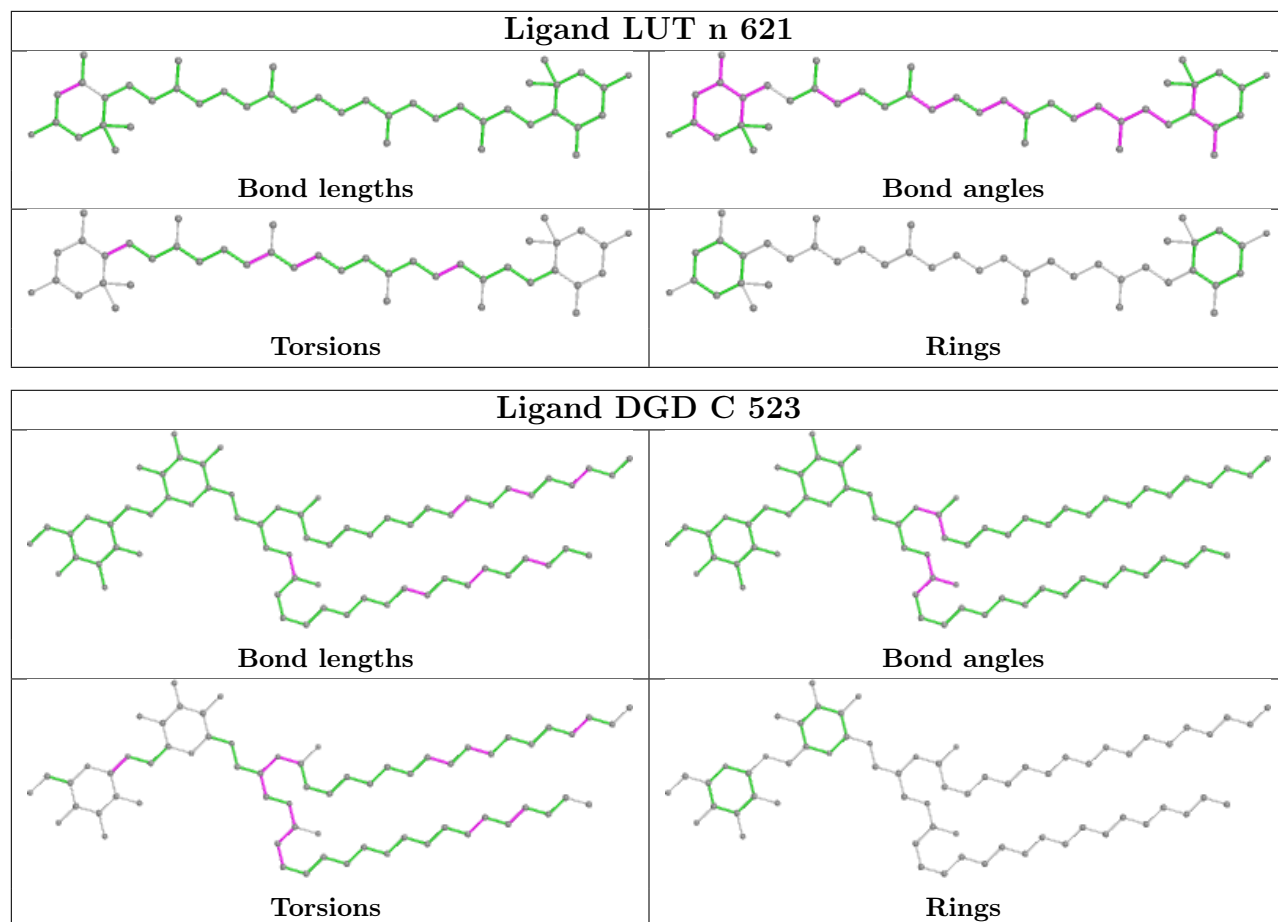


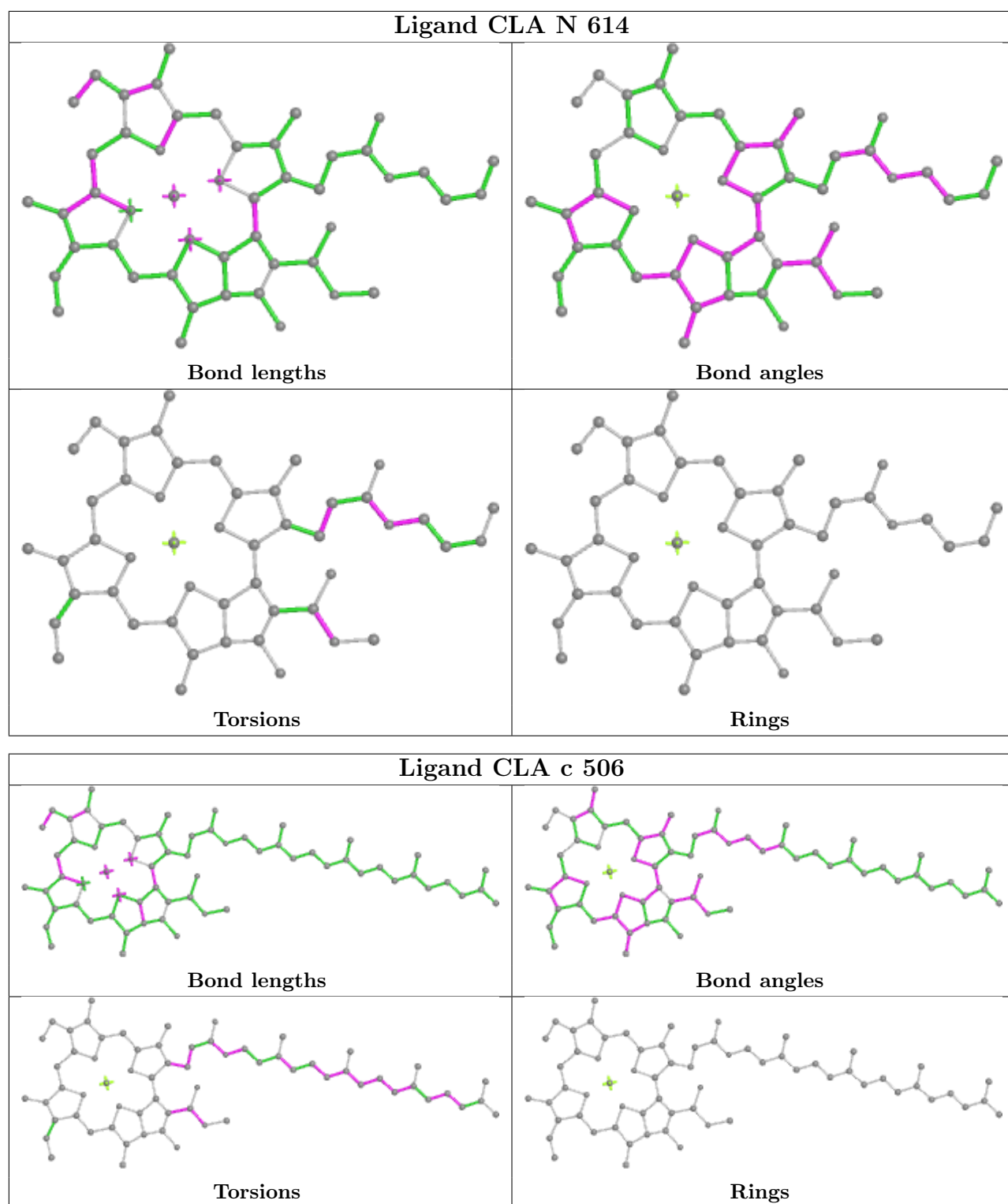




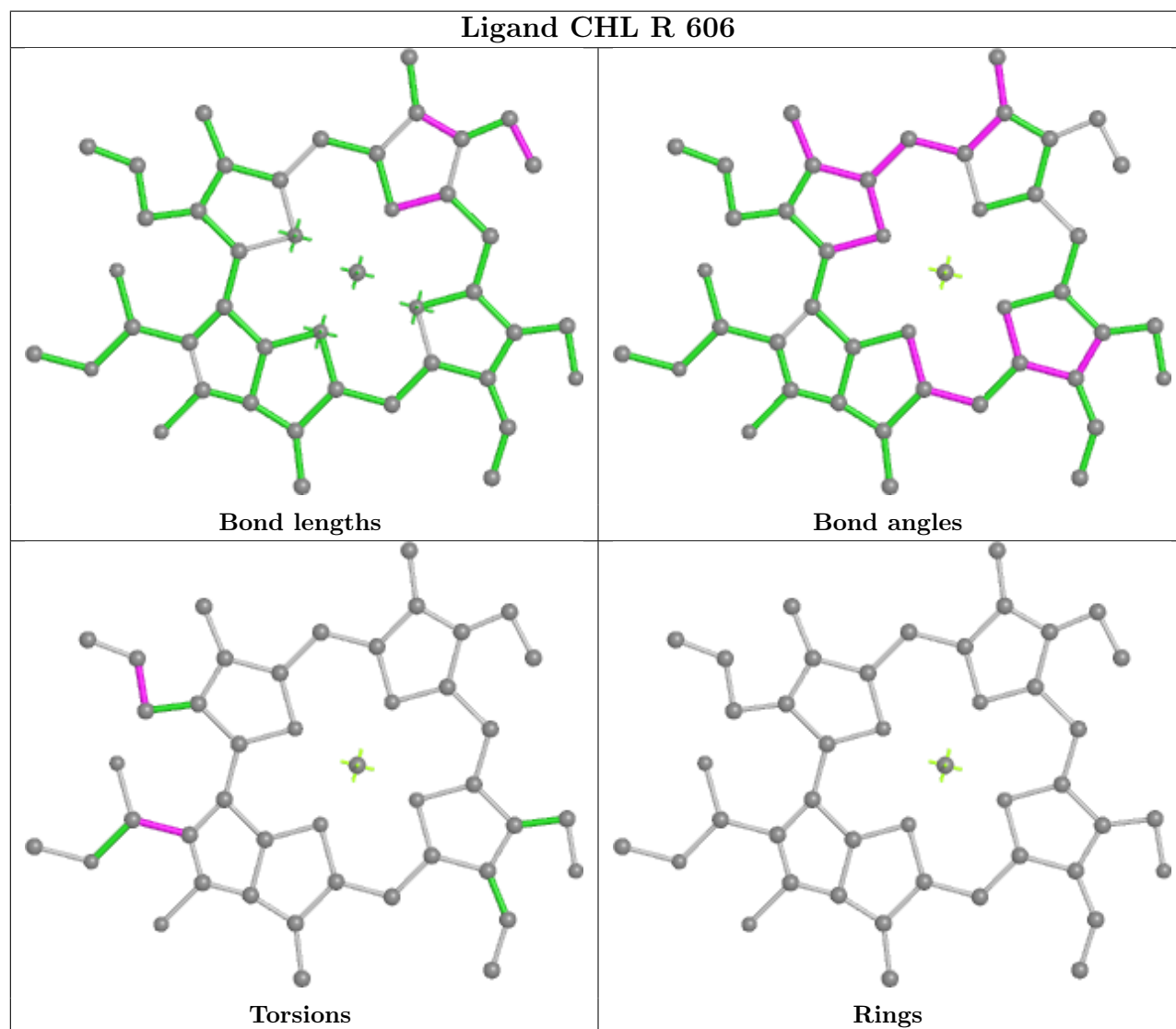
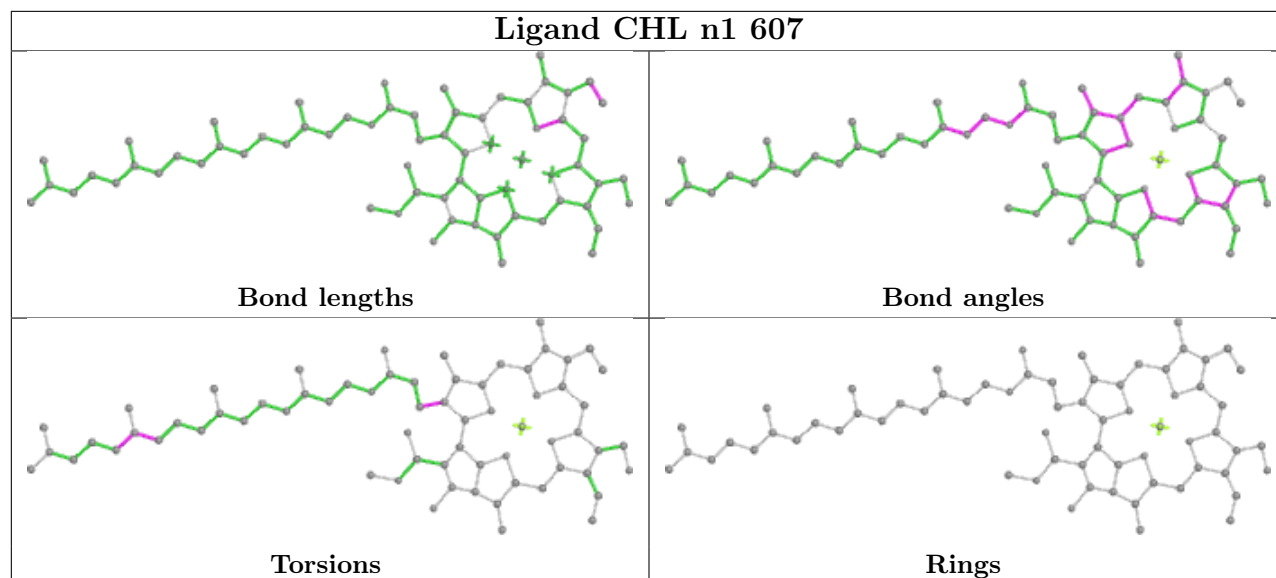


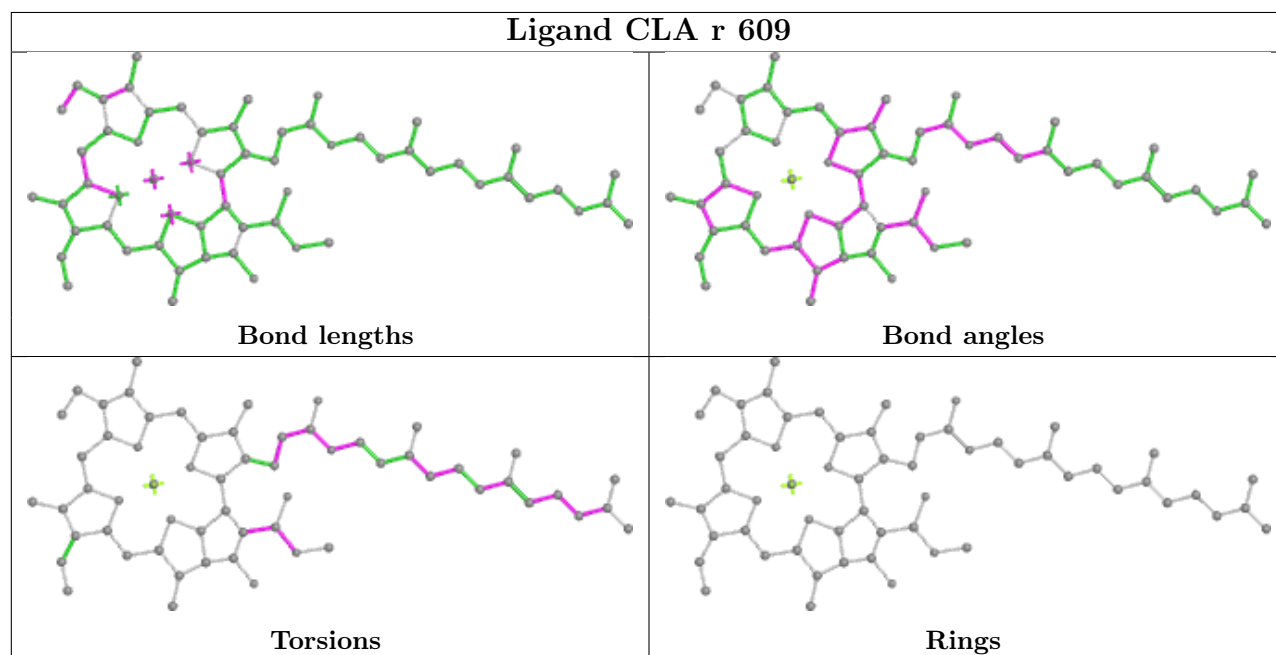
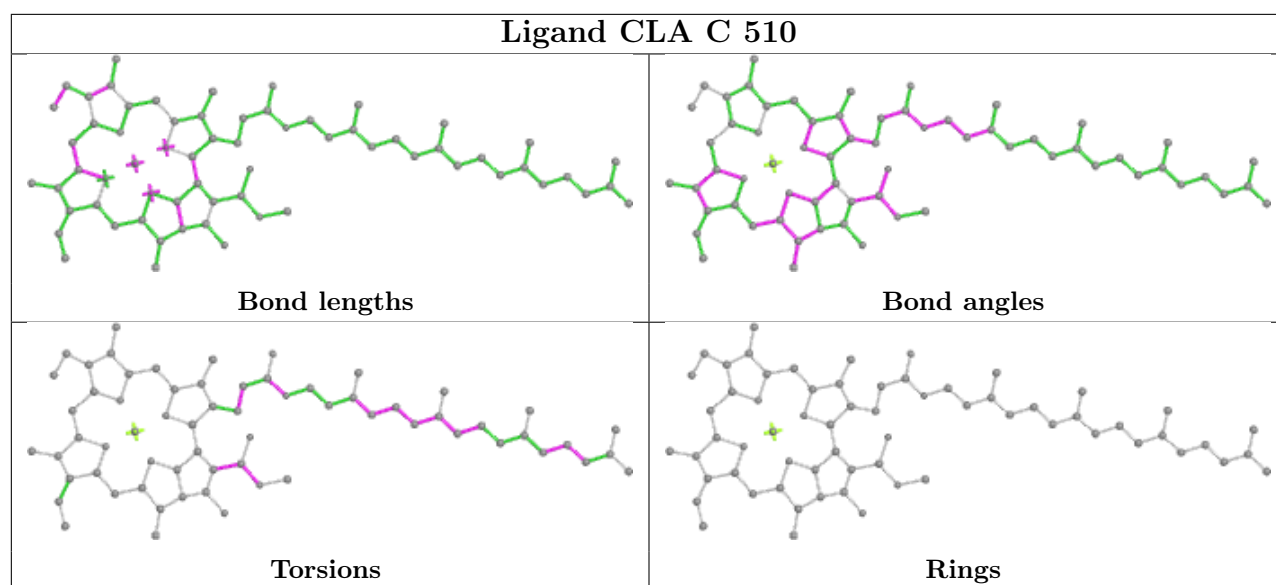


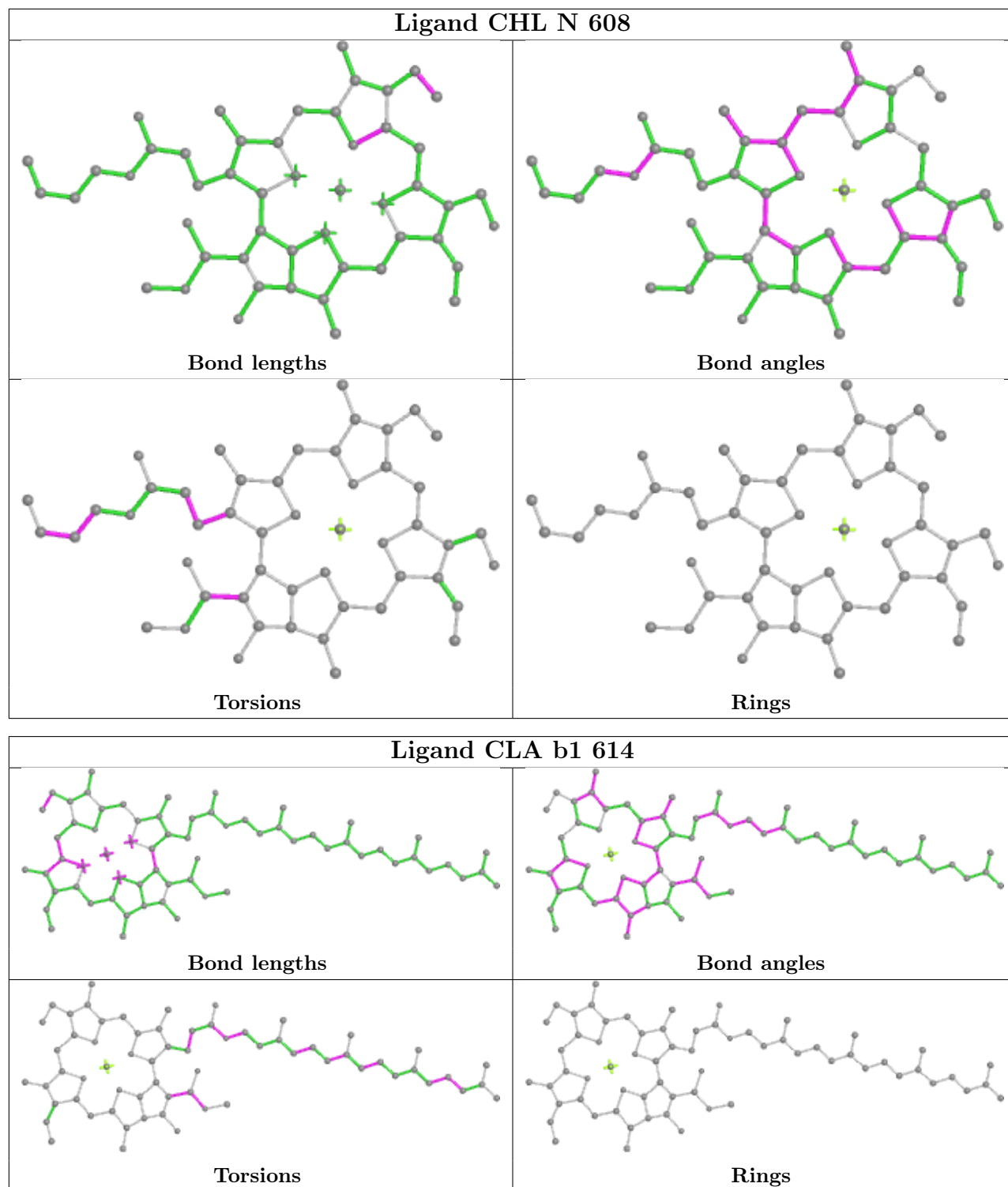


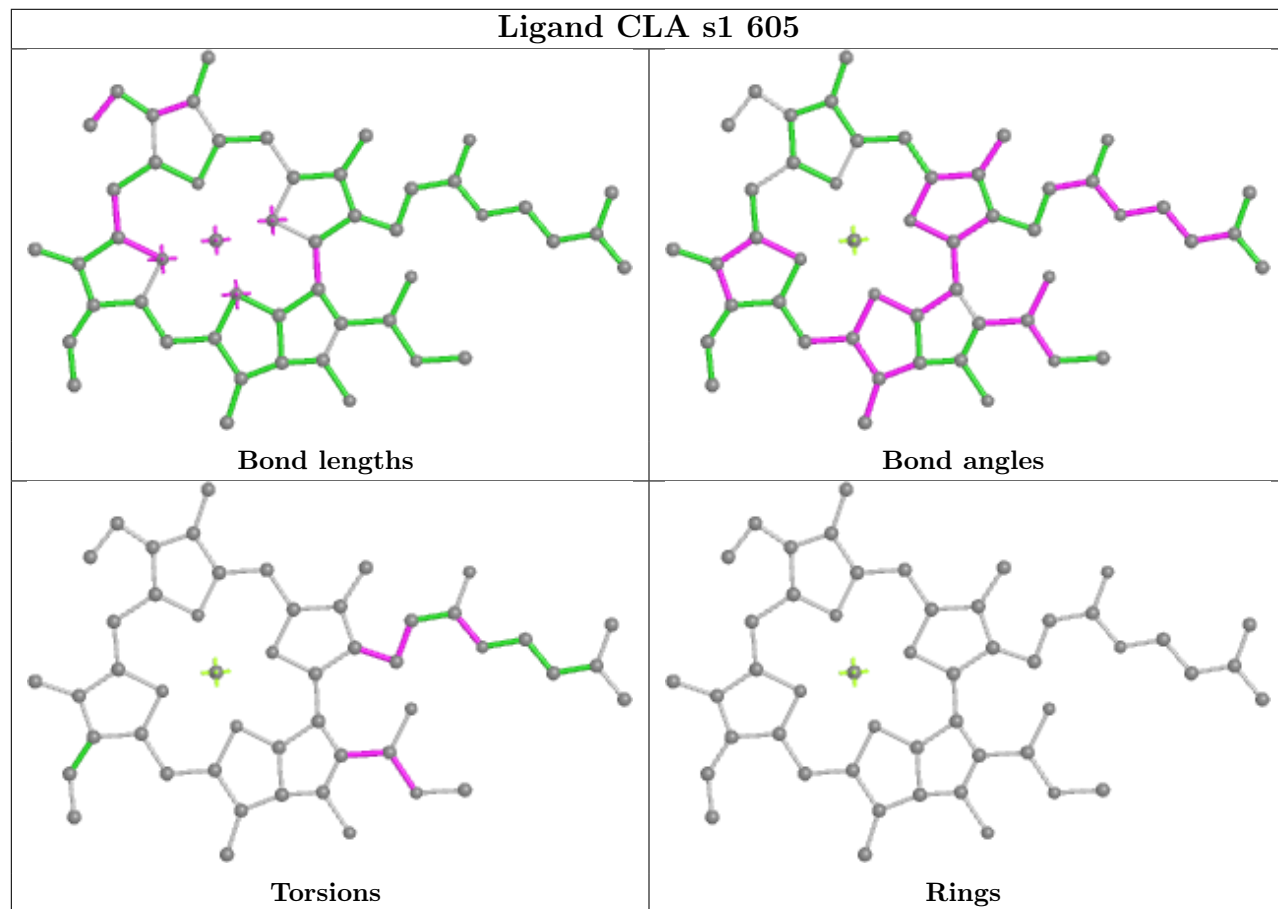
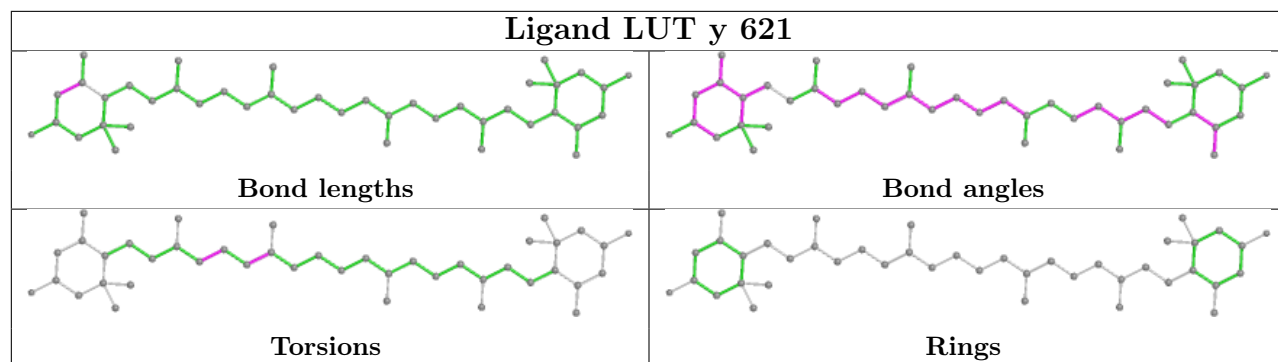


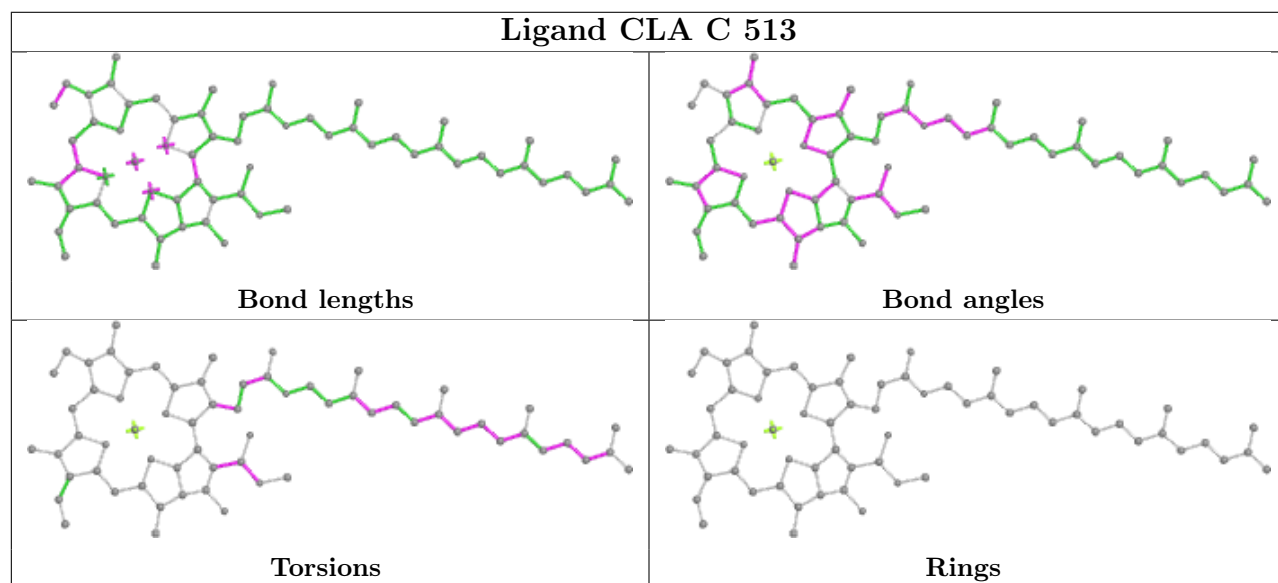
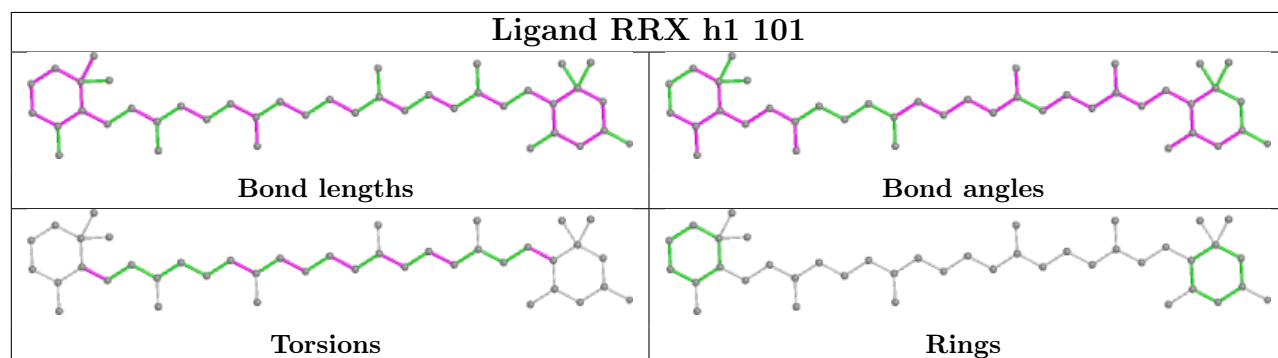
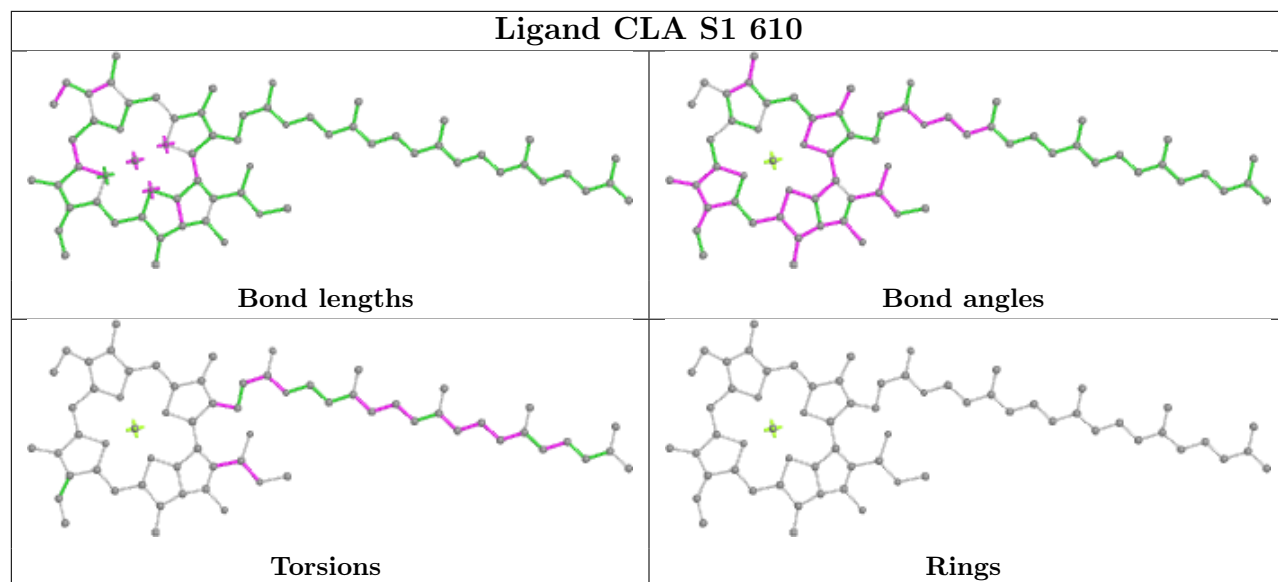


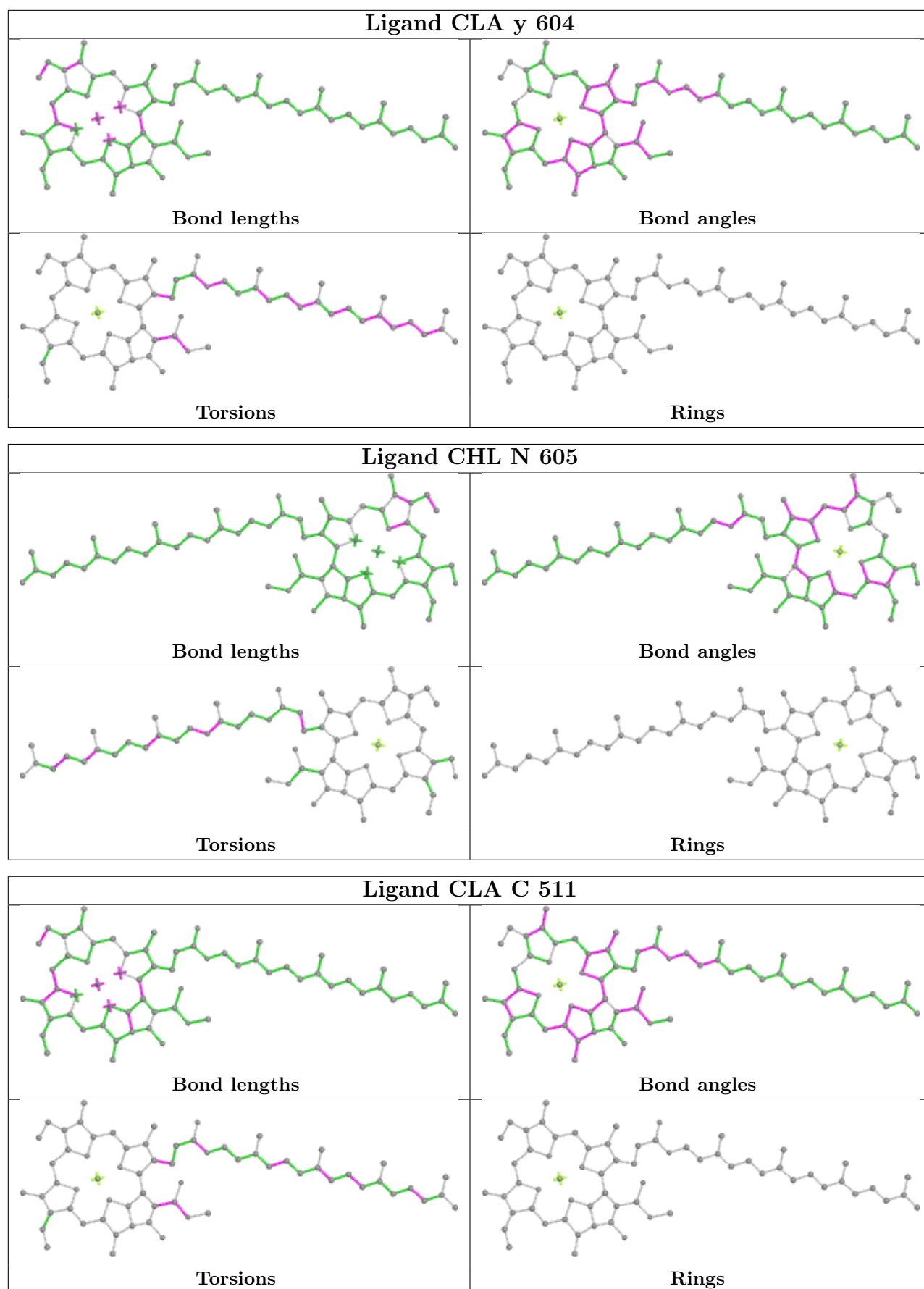


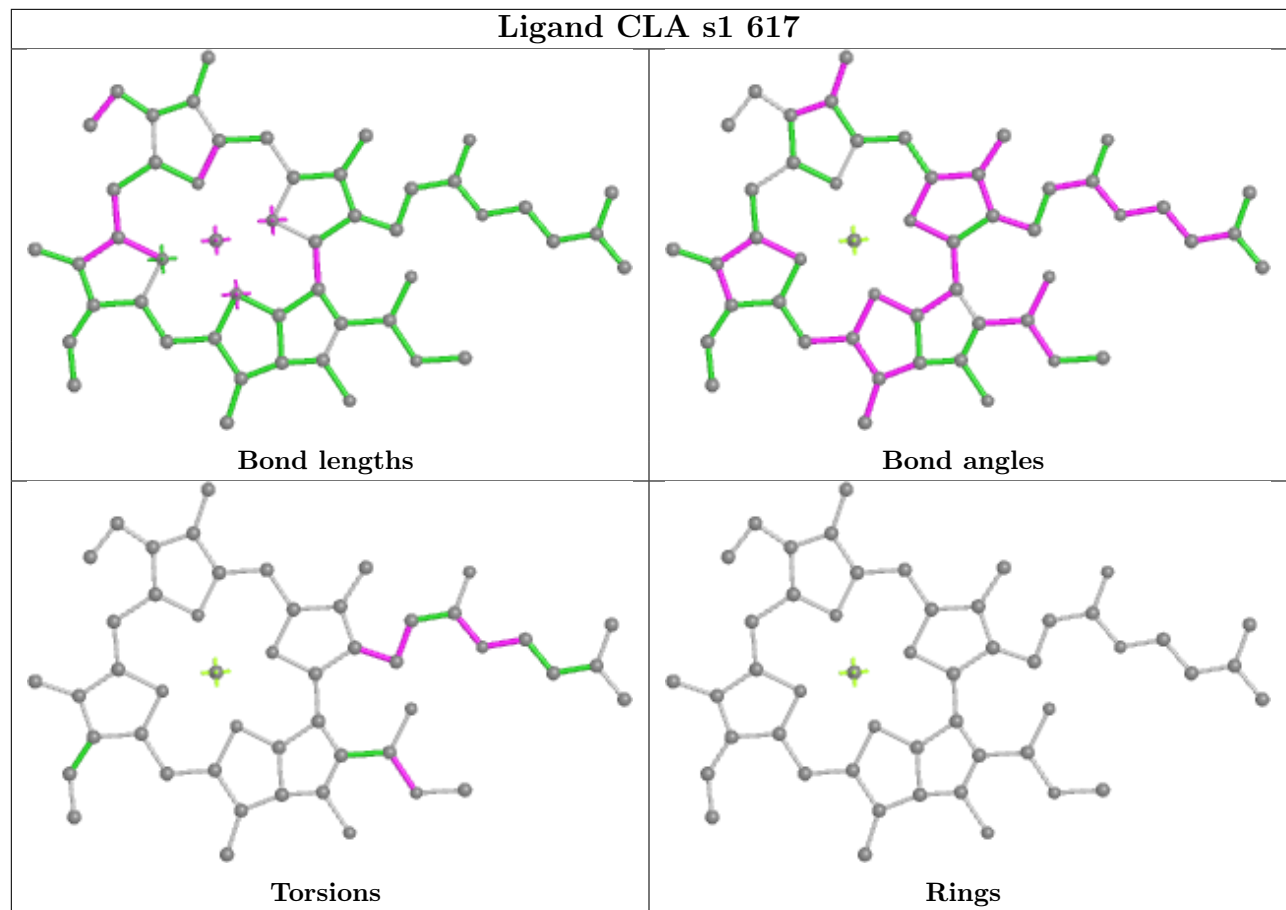


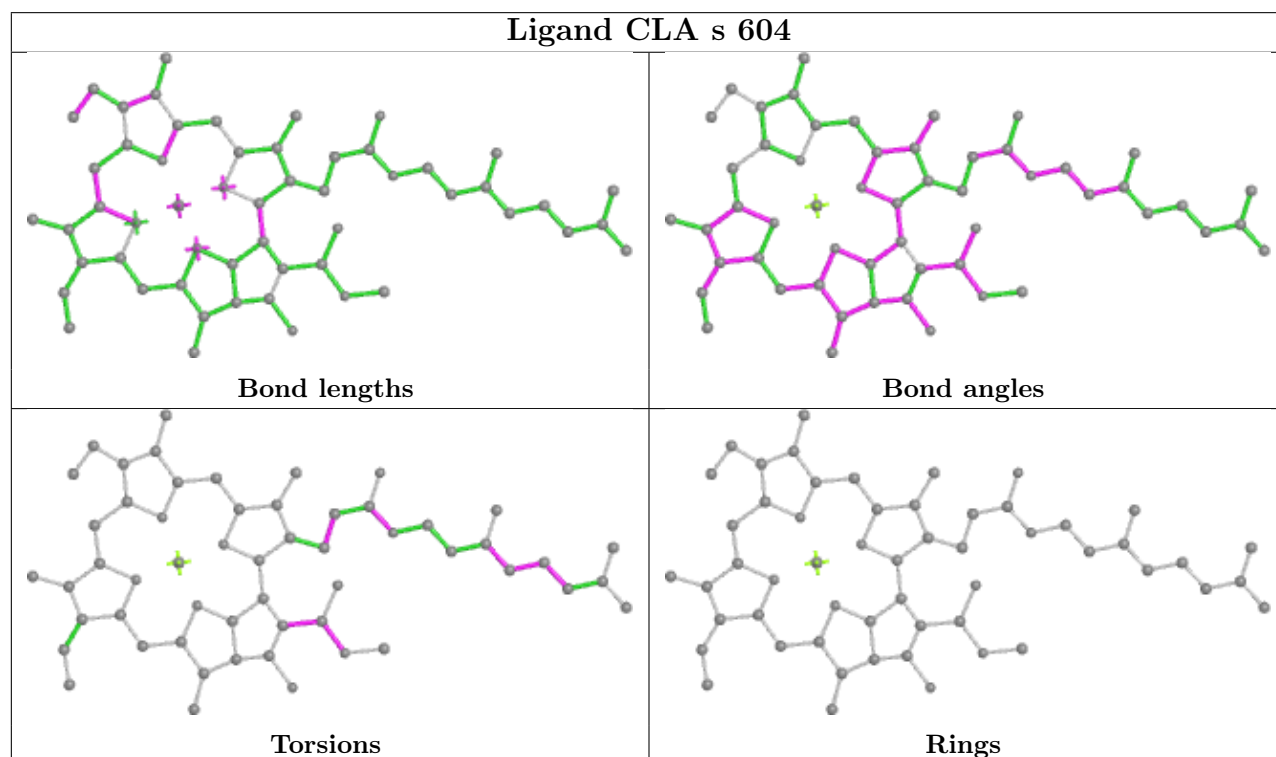
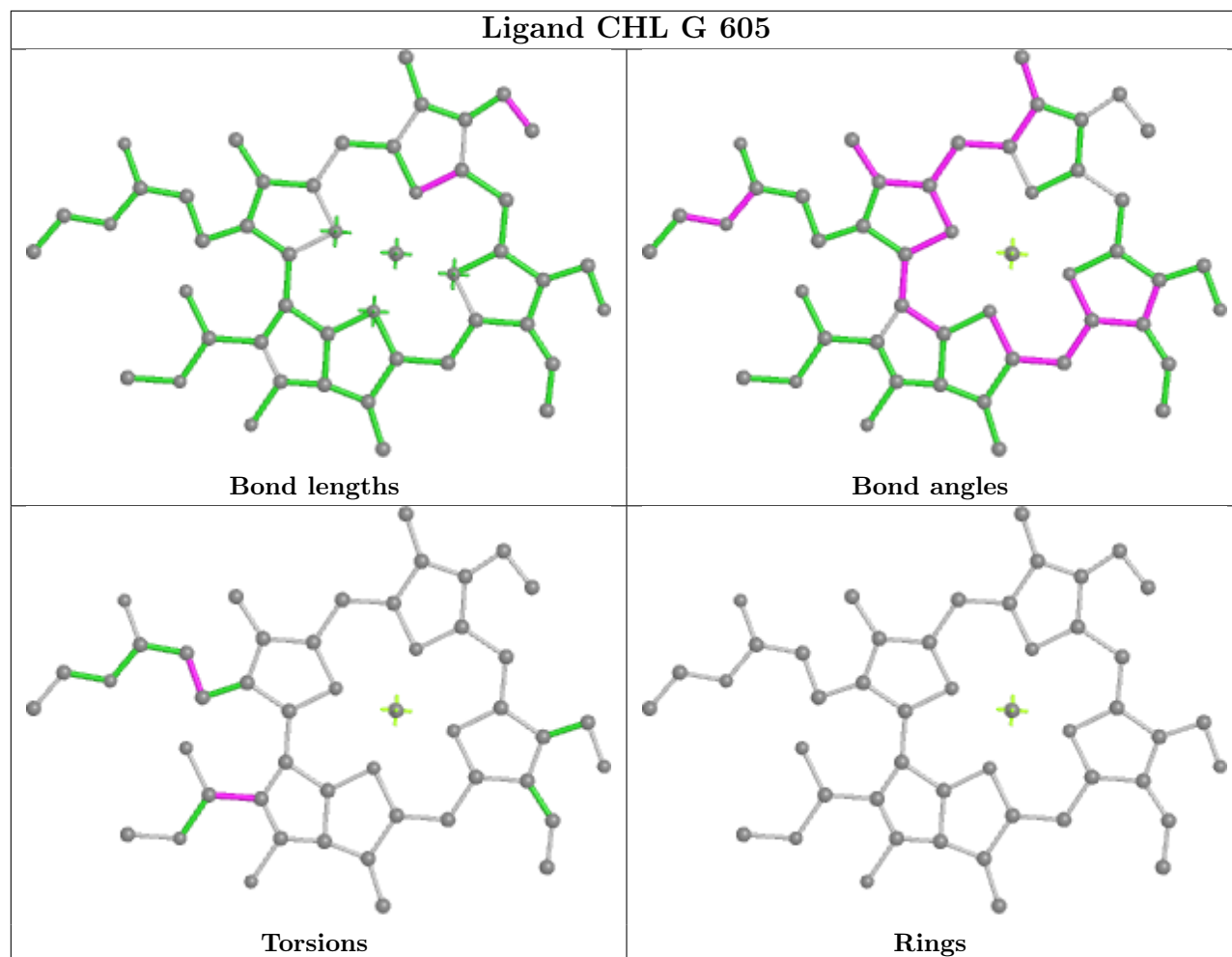




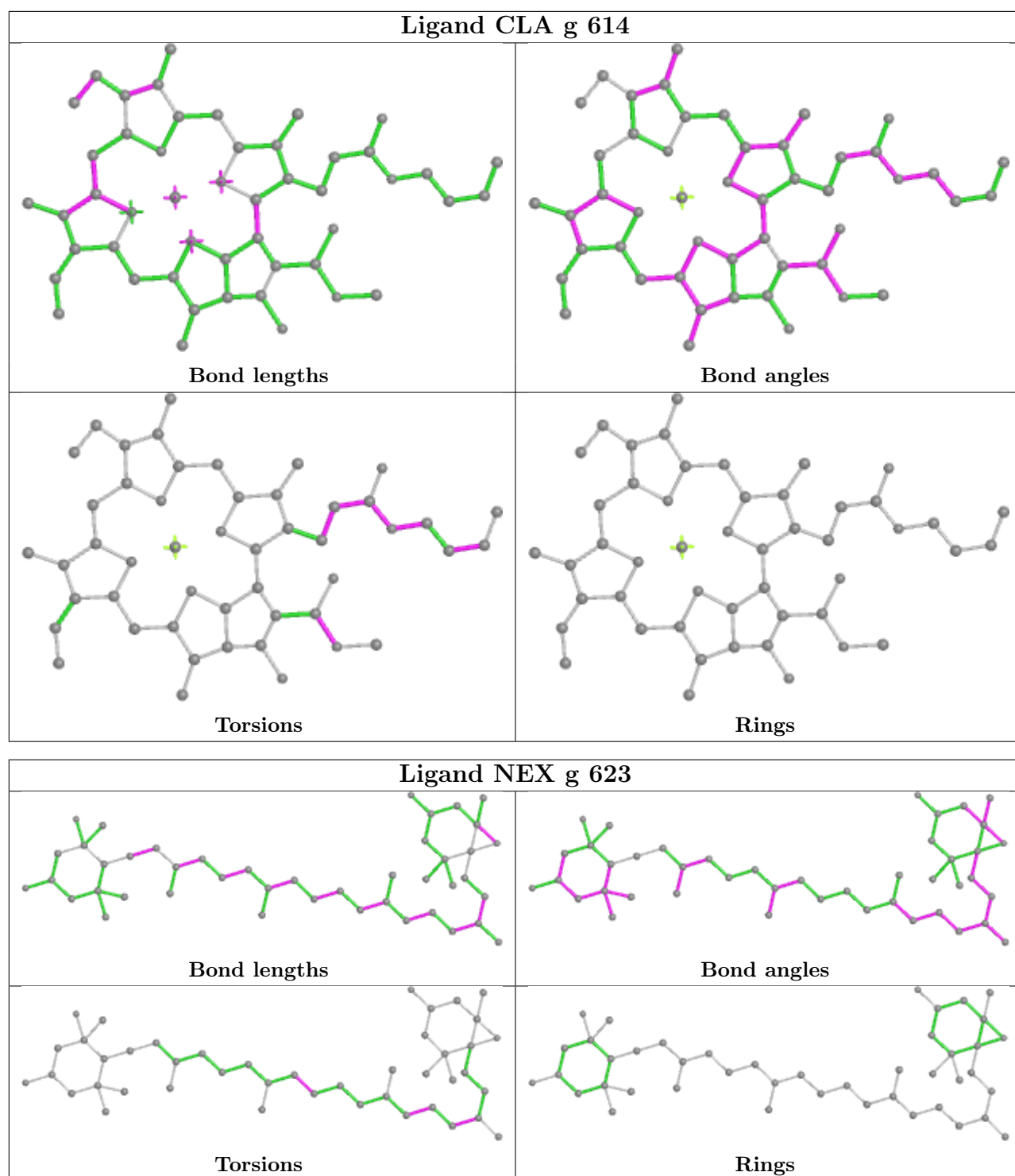


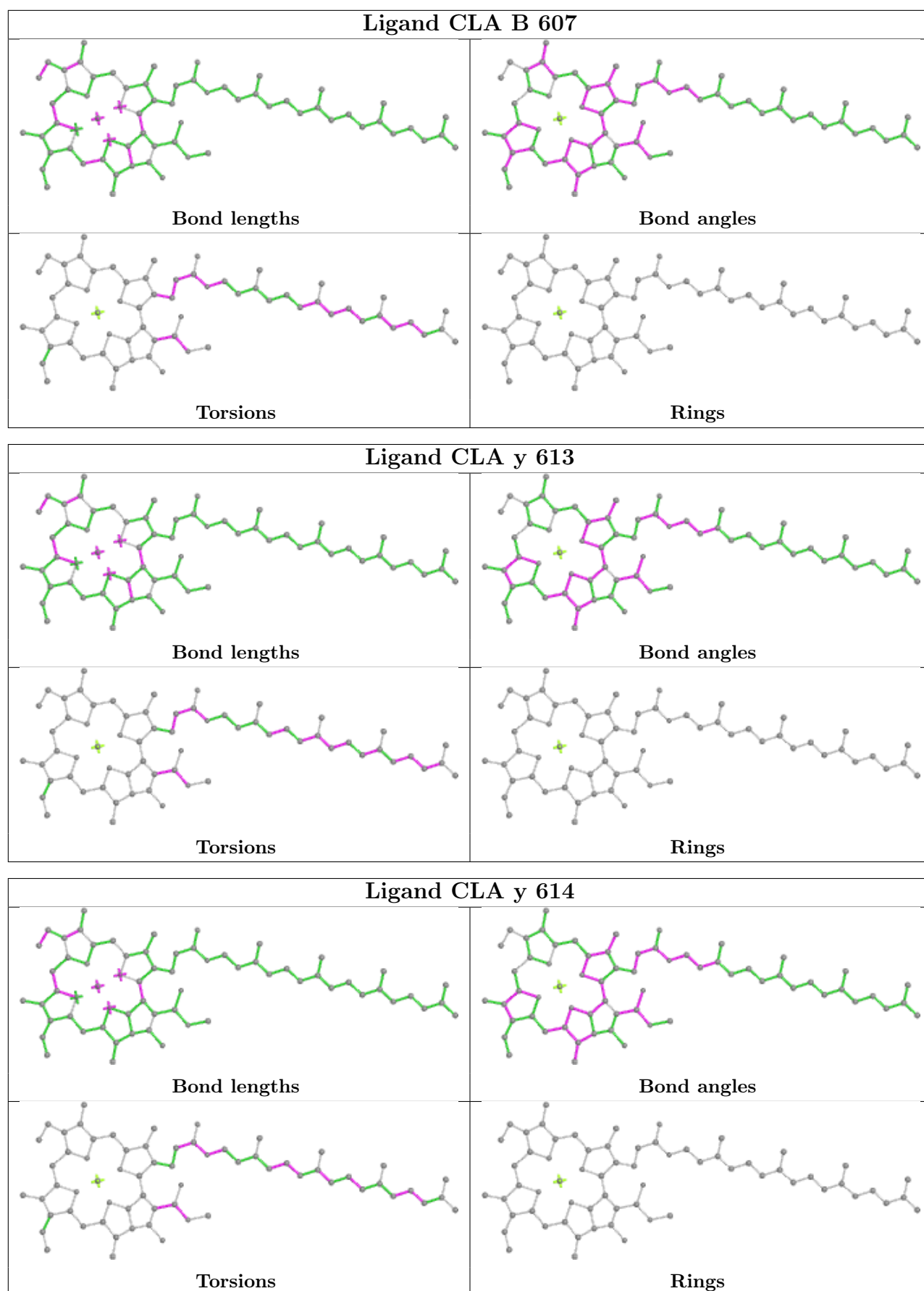


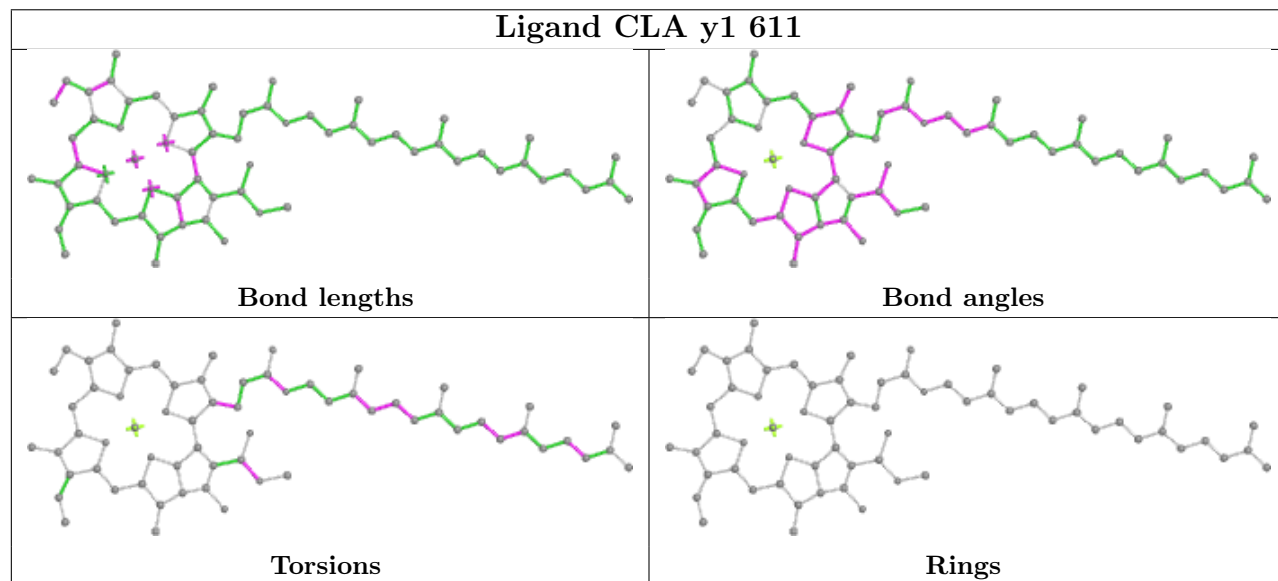
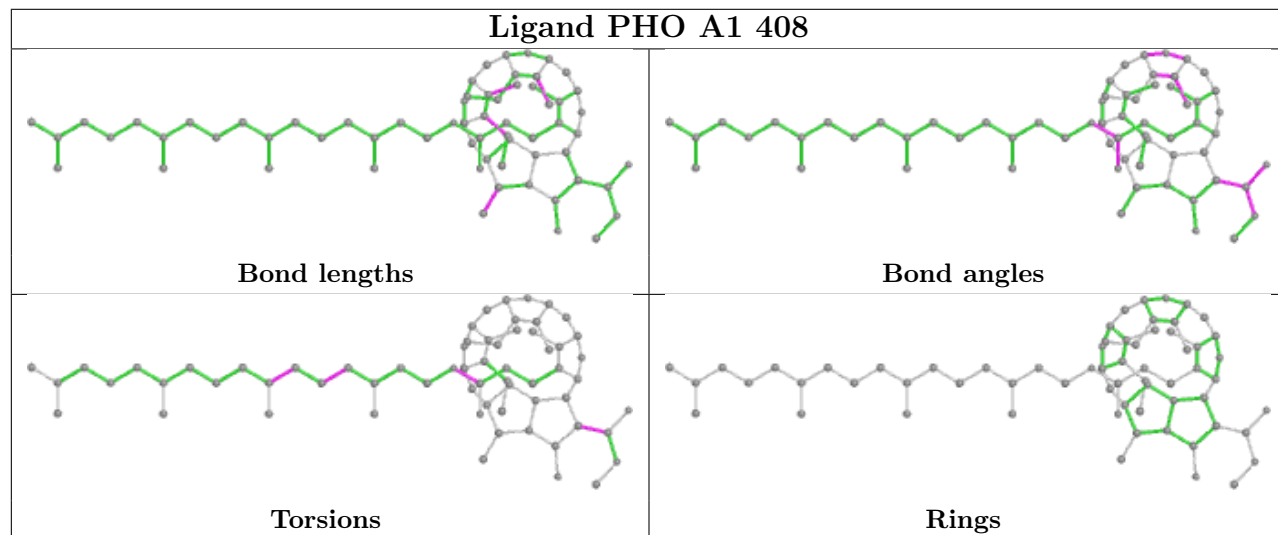
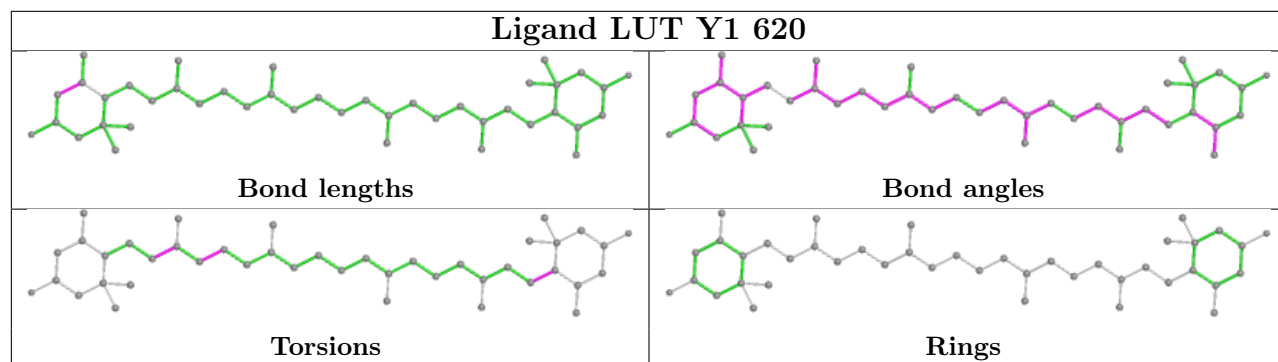


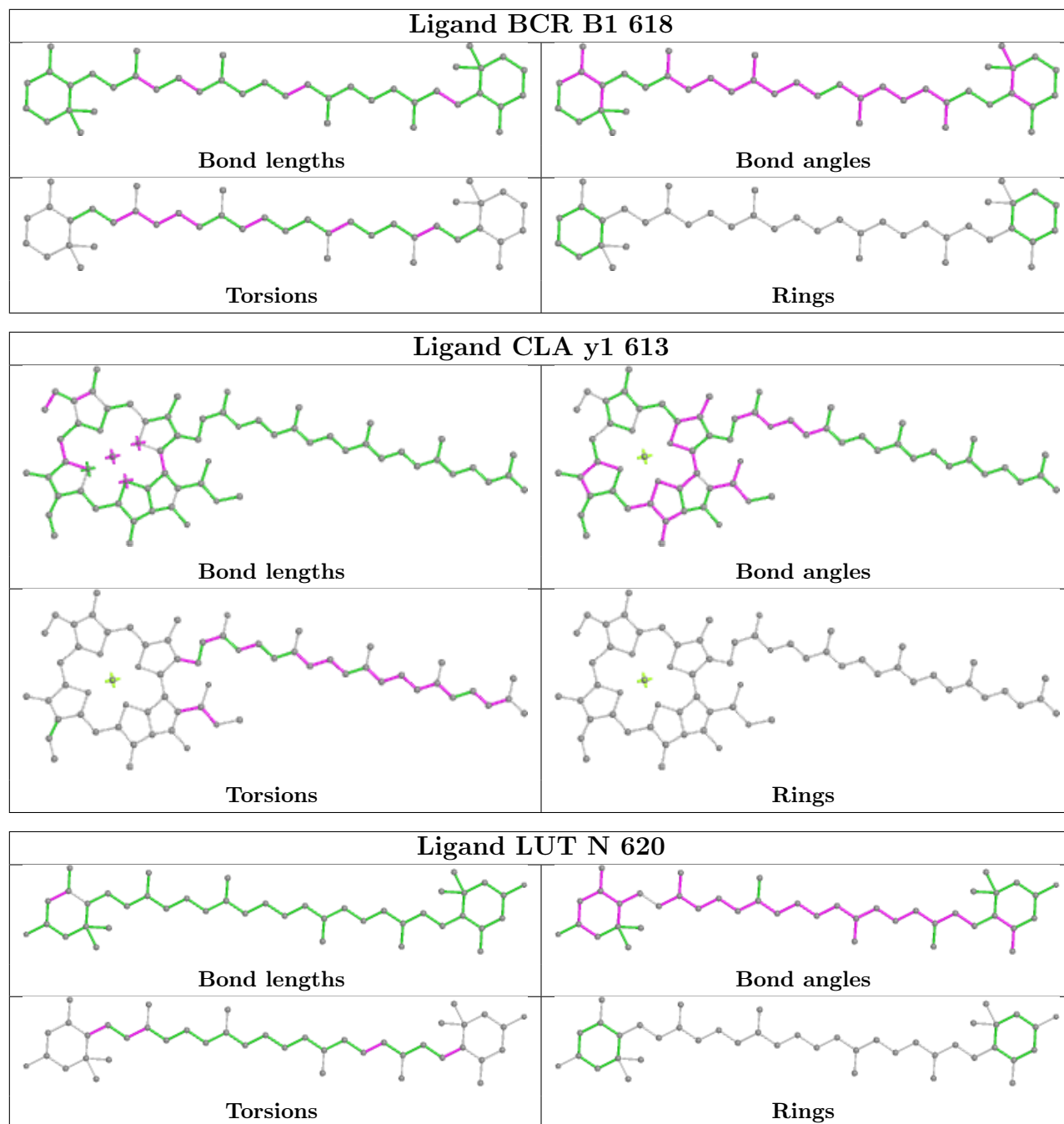


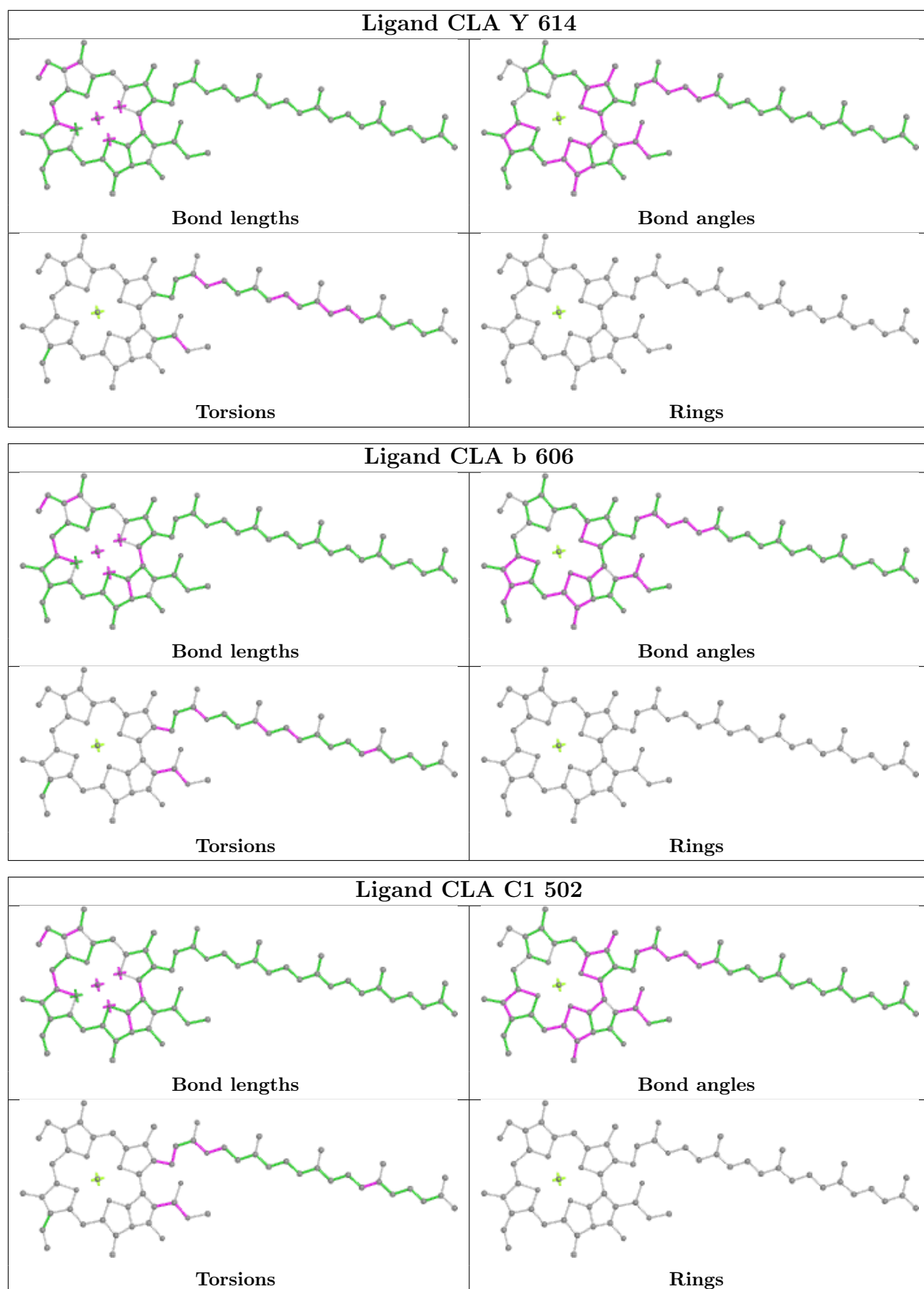












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	R	1
27	r1	1
27	R1	1
23	s	1
20	n1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	18.97
1	R	110:PRO	C	126:GLU	N	18.01
1	r1	110:PRO	C	126:GLU	N	12.33
1	R1	110:PRO	C	126:GLU	N	11.82
1	s	285:ARG	C	286:VAL	N	3.41
1	n1	57:PRO	C	58:PRO	N	3.28

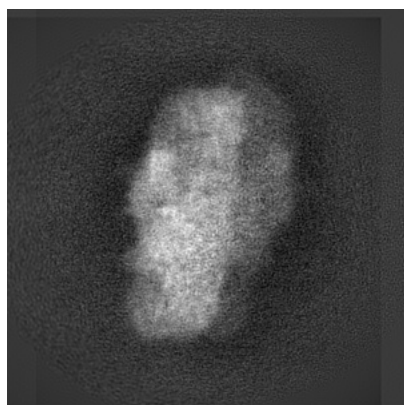
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13455. These allow visual inspection of the internal detail of the map and identification of artifacts.

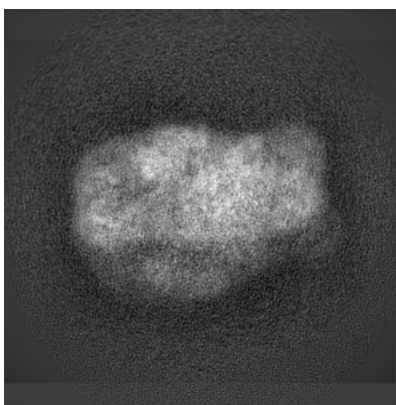
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

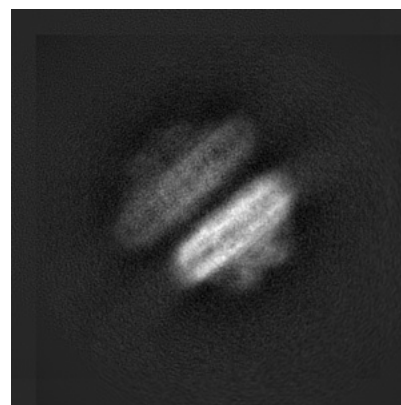
#### 6.1.1 Primary map



X



Y

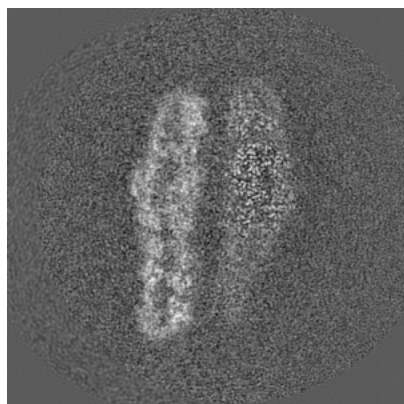


Z

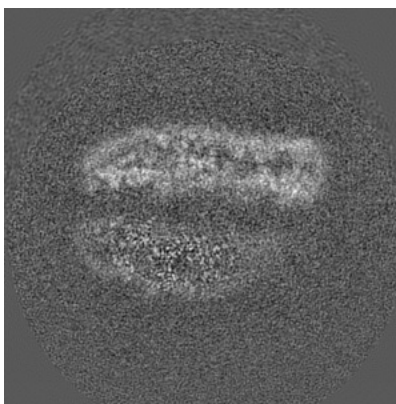
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

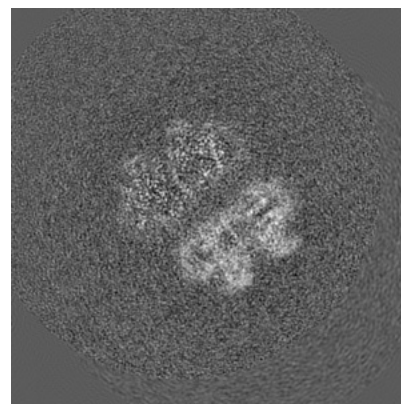
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

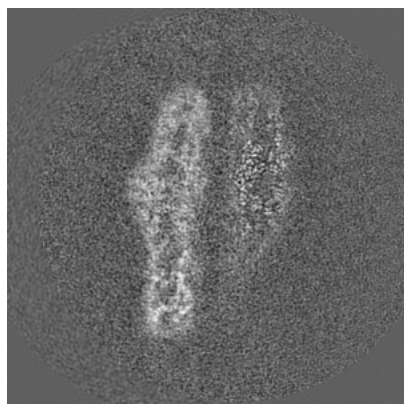


Z Index: 240

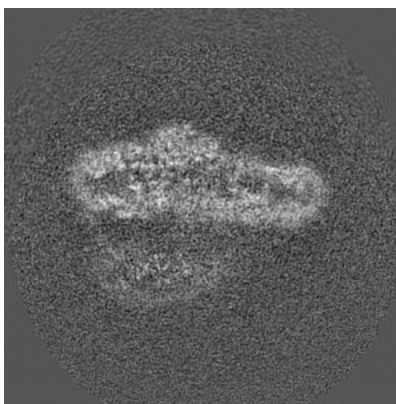
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

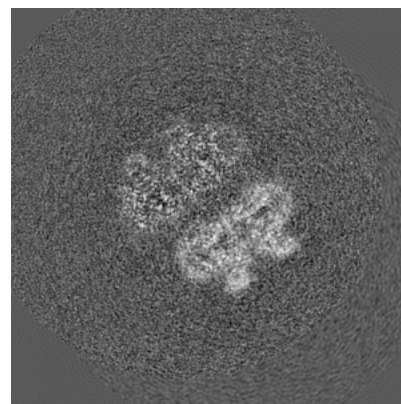
### 6.3.1 Primary map



X Index: 246



Y Index: 215



Z Index: 238

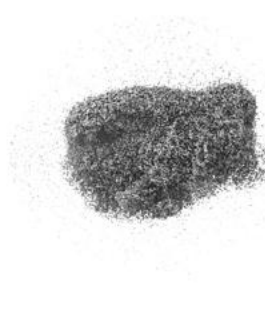
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



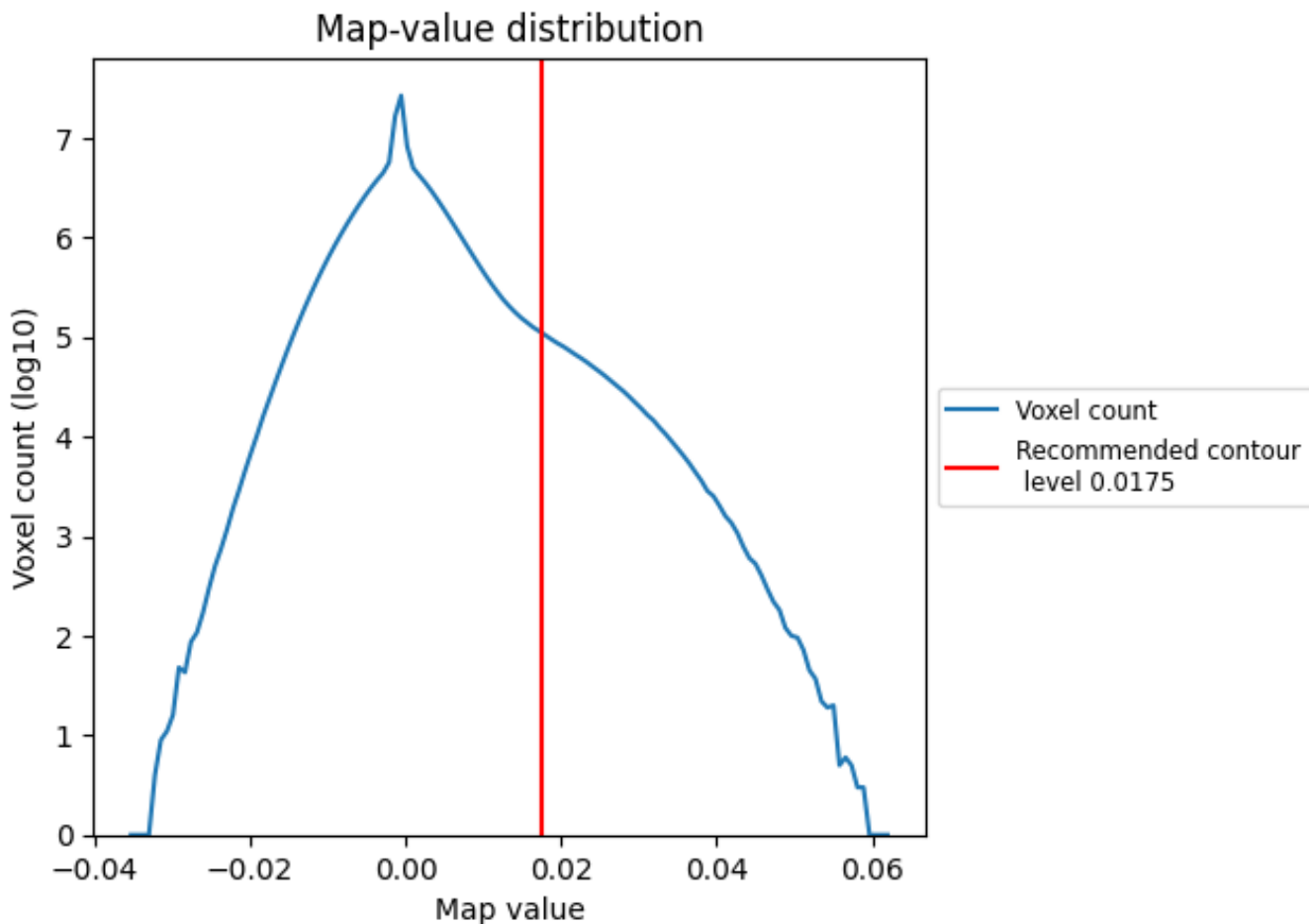
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

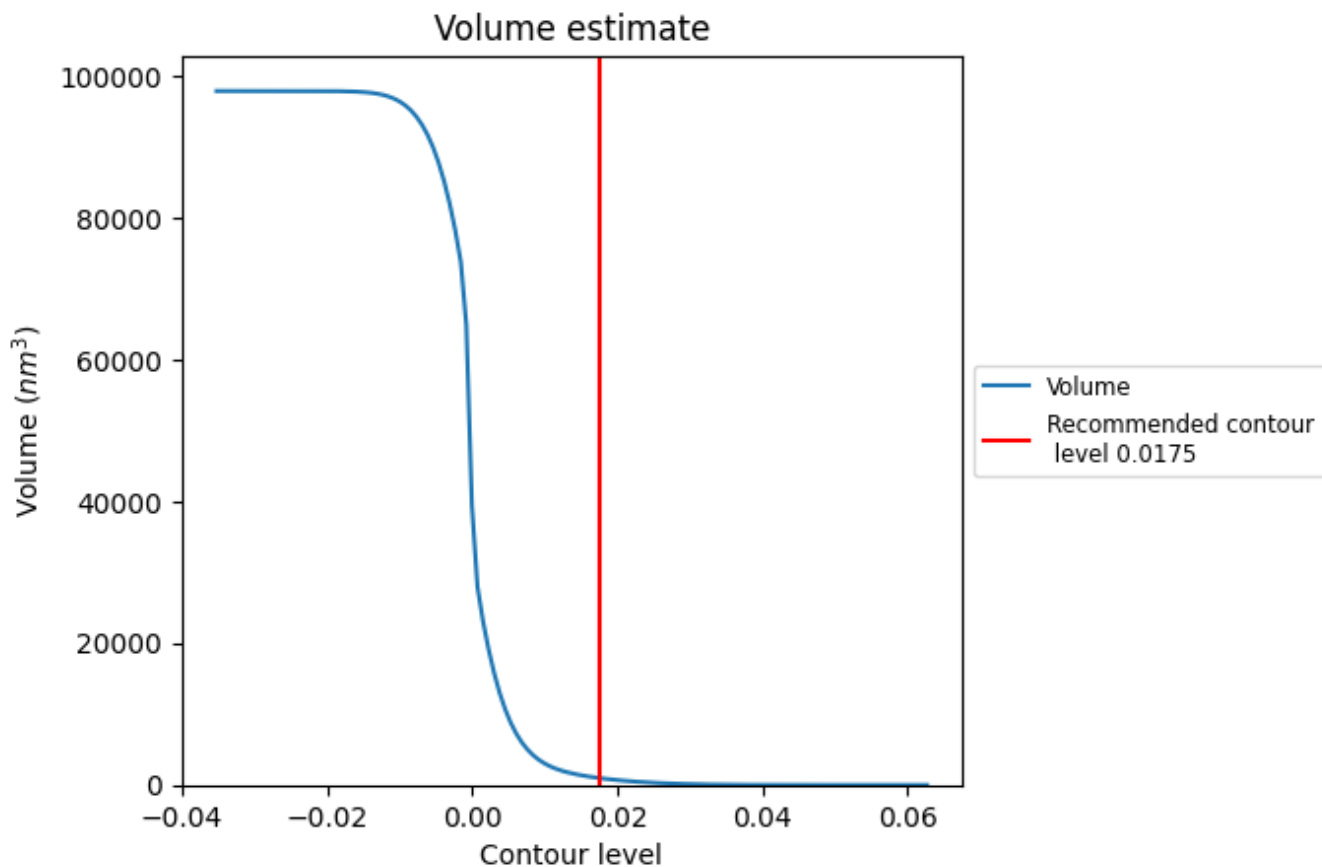
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

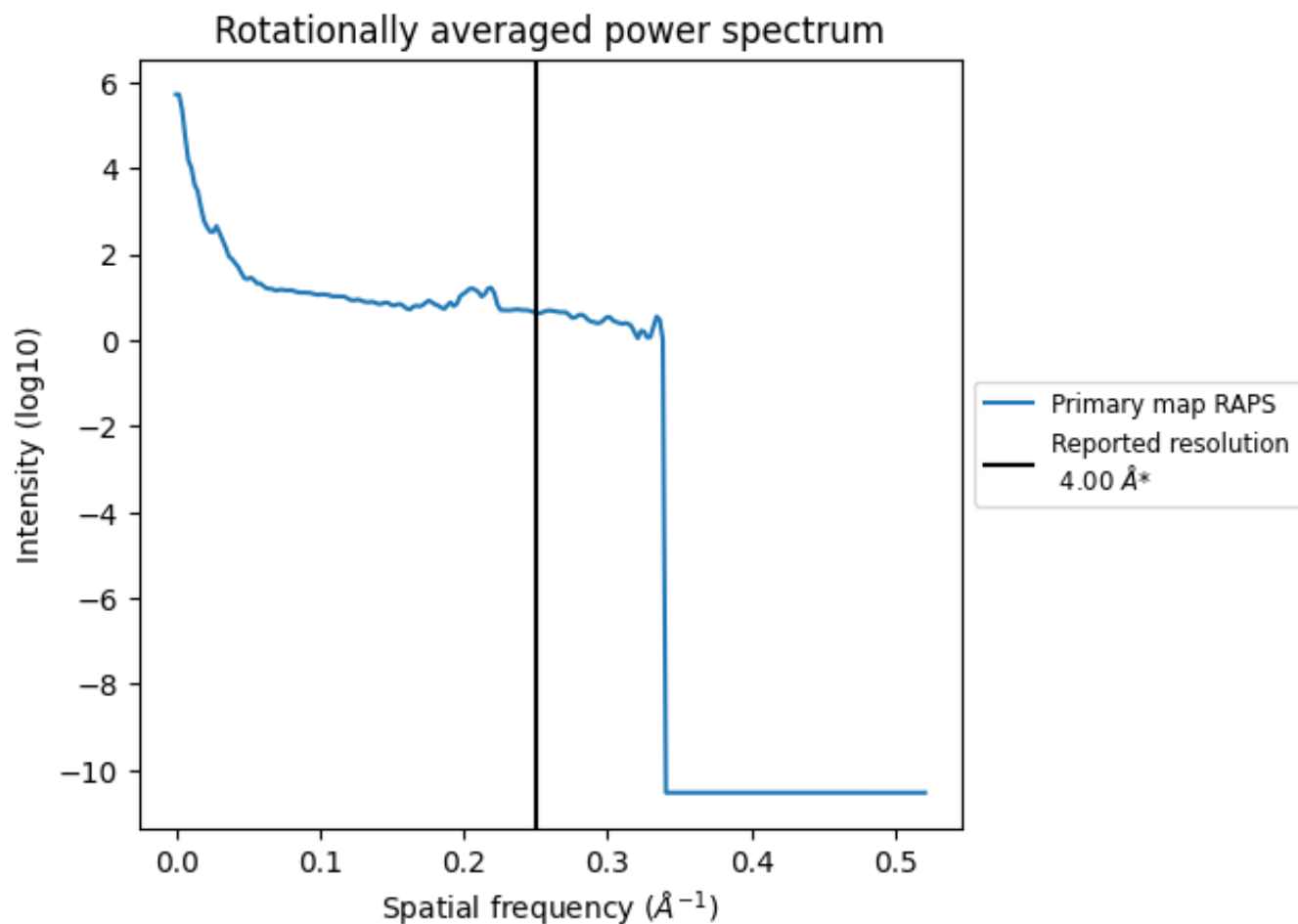
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 976  $\text{nm}^3$ ; this corresponds to an approximate mass of 881 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

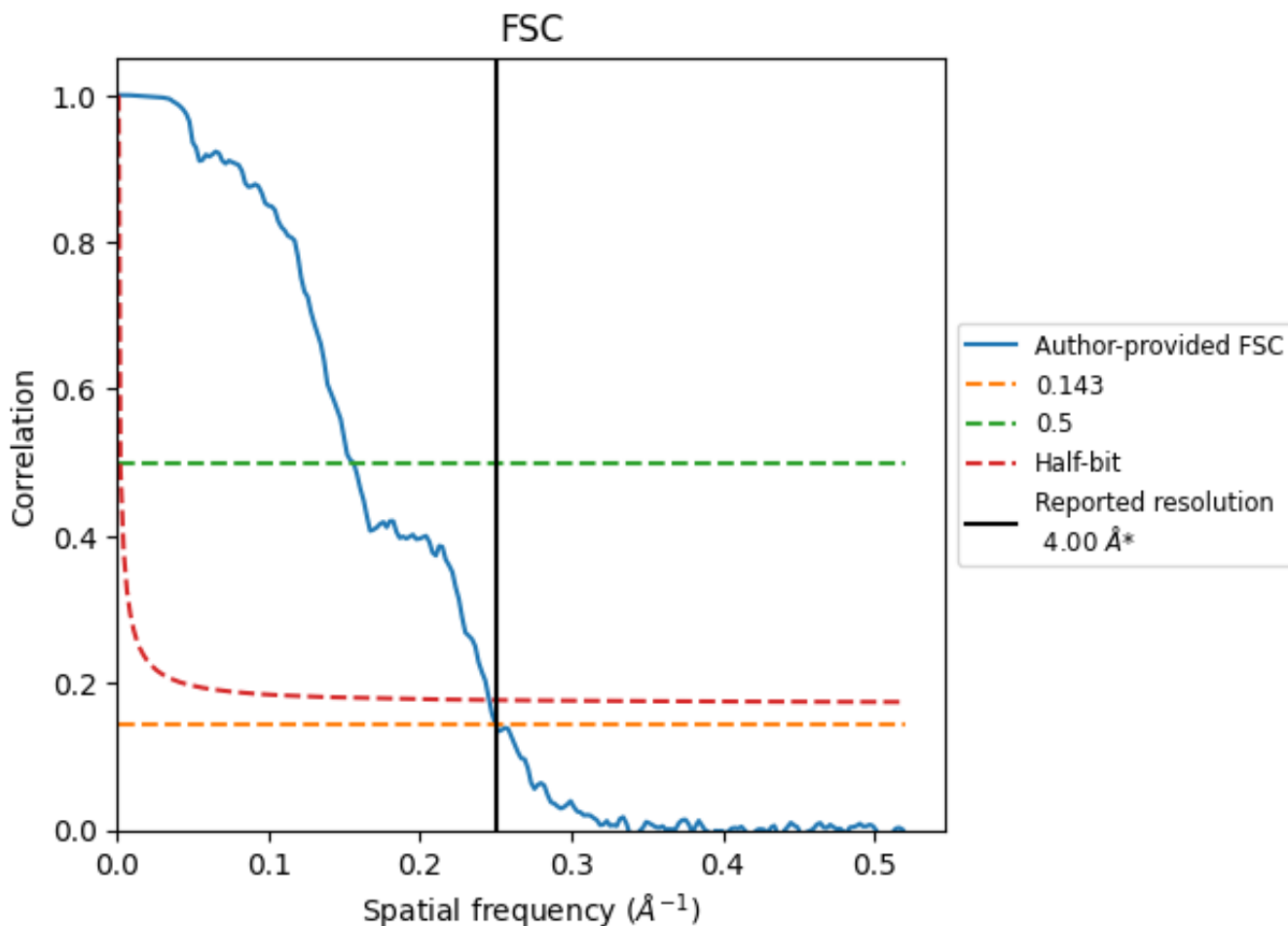


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

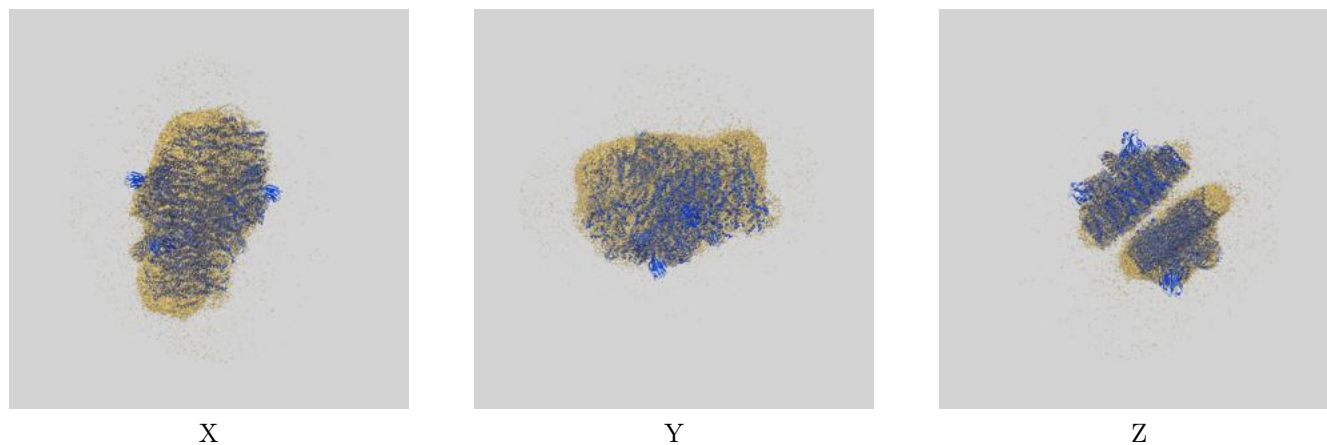
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	6.41	4.07
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13455 and PDB model 7PIW. Per-residue inclusion information can be found in section 3 on page 74.

### 9.1 Map-model overlay [i](#)

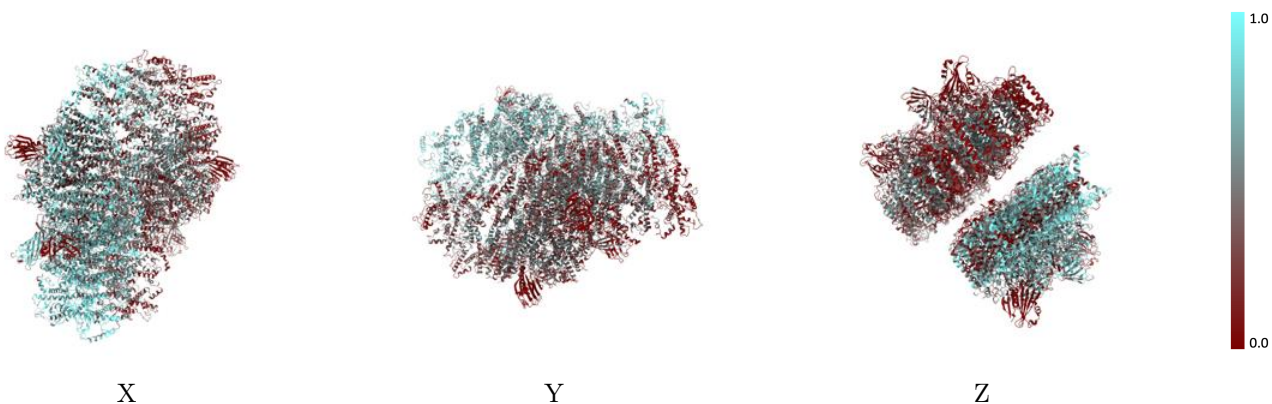


The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)

This section was not generated.

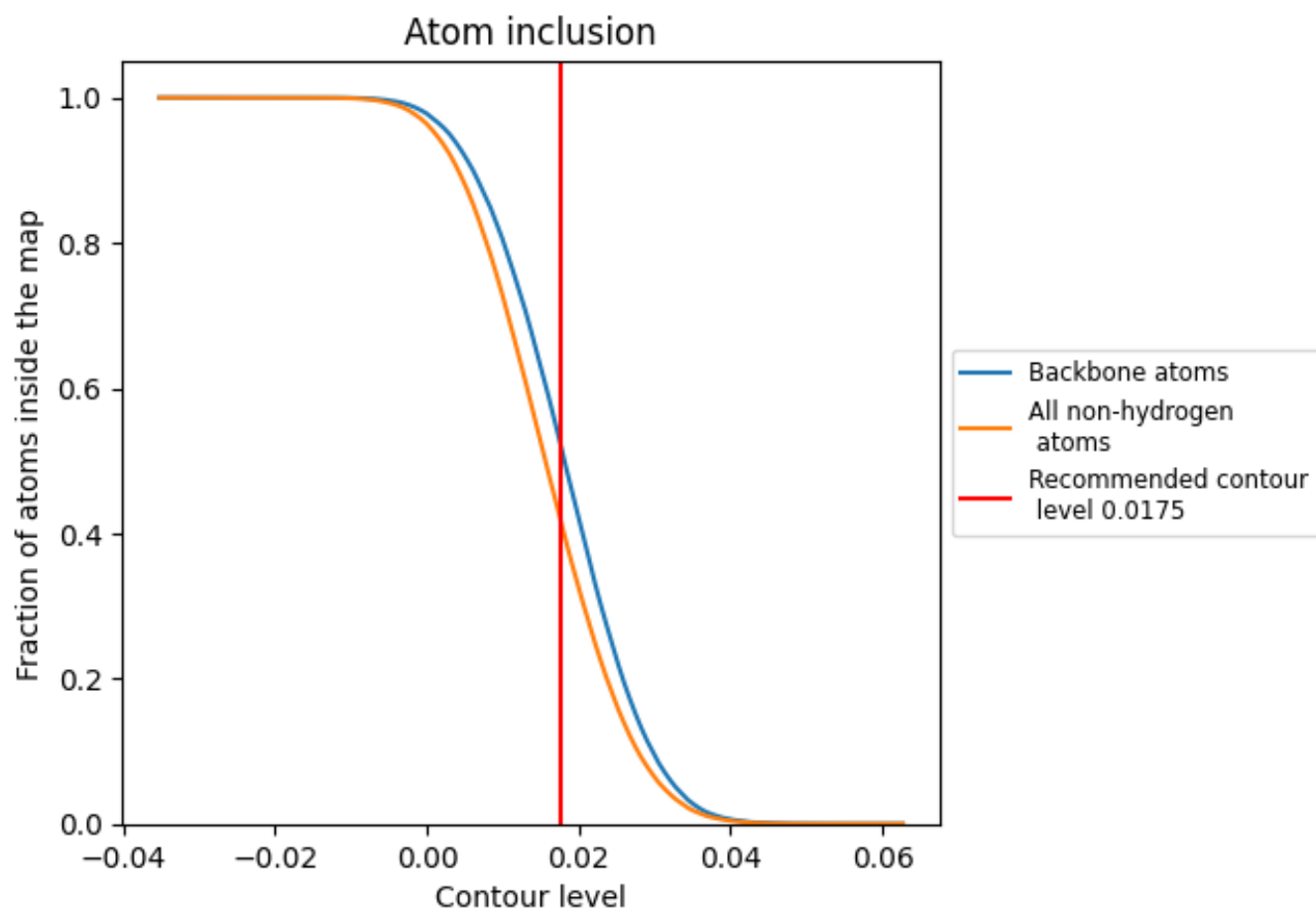
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0175).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)











































The table lists the average atom inclusion at the recommended contour level (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.4231
A	0.4924
A1	0.6122
B	0.3736
B1	0.5834
C	0.4931
C1	0.6259
D	0.4415
D1	0.5983
E	0.3812
E1	0.7459
F	0.4091
F1	0.7587
G	0.1979
G1	0.6689
H	0.2981
H1	0.5315
I	0.4674
I1	0.5398
J	0.3824
J1	0.5241
K	0.4164
K1	0.6514
L	0.3521
L1	0.4338
M	0.3306
M1	0.3818
N	0.2958
N1	0.6722
O	0.2273
O1	0.6067
P	0.0176
P1	0.0951
R	0.1040
R1	0.4664


























*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion
S	 0.2682
S1	 0.6810
T	 0.3595
T1	 0.3958
U	 0.2202
U1	 0.5413
V	 0.3600
V1	 0.6089
W	 0.3150
W1	 0.6038
X	 0.2687
X1	 0.6269
Y	 0.3619
Y1	 0.6266
Z	 0.2725
Z1	 0.6527
a	 0.4668
a1	 0.4716
b	 0.3612
b1	 0.4934
c	 0.3995
c1	 0.4770
d	 0.4389
d1	 0.4441
e	 0.2426
e1	 0.4653
f	 0.3671
f1	 0.5455
g	 0.1416
g1	 0.5719
h	 0.2436
h1	 0.4566
i	 0.4503
i1	 0.4144
j	 0.2451
j1	 0.4379
k	 0.3481
k1	 0.4057
l	 0.3915
m	 0.2479
m1	 0.3745
n	 0.1661

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion
n1	 0.5485
o	 0.2178
o1	 0.5320
p	 0.0077
p1	 0.0859
r	 0.1200
r1	 0.4777
s	 0.1607
s1	 0.4603
t	 0.3595
t1	 0.3090
u	 0.2064
u1	 0.4128
v	 0.2089
v1	 0.3333
w	 0.3364
w1	 0.4699
x	 0.2587
x1	 0.3831
y	 0.3305
y1	 0.5281
z	 0.1604
z1	 0.4242